Spectral Fitting in AXAF Calibration Detectors

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ABSTRACT

We discuss details of the spectral fitting procedures and algorithms used in deriving line count rates for the calibration of AXAF (the Advanced X-ray Astrophysics Facility) during end-to-end testing in the winter and spring of 1996/1997. An approach involving simultaneously fitting both detector and source parameters was implemented within XSPEC, a standard x-ray spectral fitting package (Arnaud 1996).

Theoretical and practical difficulties in fitting spectra taken with Flow Proportional Counters (FPC) and Solid State Detectors (SSD) will be discussed, including both effects incorporated into the numerical model, and those which must be estimated outside the model.

Sensitivity of the parameter of interest, the counts in a strong line in the spectrum, to changes and errors in the other fit parameters is explored. The impact of uncertainties on the overall absolute AXAF calibration is discussed.

Keywords: X-ray optics, Wolter Type-I, AXAF, Calibration, Spectral Fitting

1. INTRODUCTION

During the time period from 1996 December 18 through 1997 April 25, an extensive ground calibration was conducted on many of the components of the Advanced X-ray Astrophysics Facility (AXAF), the next in the series of NASA's Great Observatories. The systems tested include the High Resolution Mirror Assembly (HRMA), the Objective Gratings, and the two flight science instruments, the ACIS (AXAF CCD Imaging Spectrometer), and the HRC (High Resolution Camera).

Phase I of the calibration program consisted of a calibration of the HRMA and the Gratings using non-flight x-ray detectors. In Phase II of the program, the science instruments were calibrated with the HRMA and Gratings, forming an end-to-end test of the telescope essentially in the flight configuration. We report here on the Phase I HRMA calibration, and in particular on the role that spectral fitting plays in that calibration, and in assessing the uncertainties.

The X-Ray Calibration Facility (XRCF) at Marshall Space Flight Center (MSFC) in Huntsville, Alabama, consists of a large vacuum tank to contain the mirror and detectors, connected to an evacuated tube over 500 m long. At the other end of the tube is an array of x-ray sources, including an electron impact point source (EIPS), two monochromators, and a Penning source.

The Phase I detectors in use were those of the HRMA X-ray Detector System (HXDS). These SAO-provided detectors include seven nearly identical flow proportional counters (FPC), two germanium solid state detectors (SSD), and one microchannel plate camera known as the High Speed Imager (HSI). They are arranged as follows: two of the FPCs, one SSD, and the HSI are on translation stages at the focal point of the mirror. The FPCs and SSD have selectable apertures, and the whole assembly can be positioned in three dimensions to within about 2 μm of the

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desired location. Four FPC detectors surround the entrance of the HRMA; these are known as Beam Normalization Detectors at the HRMA (BND-H). One of these detectors can be moved about in the beam to measure the spatial uniformity of the x-ray beam at the telescope entrance. The remaining FPC and SSD are located much closer to the source, and can likewise be used to monitor the beam's temporal and spatial uniformity.

A typical HRMA calibration experiment consists of exposing a focal plane instrument, and the complete suite of six BND detectors, to an x-ray beam simultaneously. Most experiments used the electron impact point source (EIPS), because it produces a substantially higher flux of x-rays than any of the other available sources. The spectrum, however, consists of a spectral line (or more than one), whose energy depends on the composition of the anode in the source, and a Bremsstrahlung continuum, extending from low energies to the source voltage, and modified somewhat in shape by the presence of a thin filter of some material between the source and the detectors. One can measure effective areas, for example, by using the BND detectors to measure the x-ray flux at the HRMA entrance, and dividing this into the count rate in the focal plane detector. It is most meaningful to do this at a single energy, typically the energy of the spectral line in the source spectrum.

This necessitates a procedure for determining the fraction of the total measured counting rate detected which consists of spectral line photons. The procedure must be robust, accurate, stable (for example in cases of low signal-to-noise or strong continuum), and suitable for a high degree of automation (as we have over 290,000 pulse-height spectra to be fit from Phase I alone).

2. SPECTRAL DATA REDUCTION FOR AXAF CALIBRATION

The spectral data delivered by the HRMA X-ray Detector System (HXDS) consists of pulse-height spectra (*i.e.* histograms of events *vs.*pulse-height) with minimal header information containing, for example, the start time, the total exposure time, an estimate of the deadtime, versions of control software that were used, etc. Also provided are other files containing experimental details, quick region-of-interest count rates, and other pertinent information.

We have put together a model (called "JMKmod" for Jahoda-McCammon Kramer model) for the XSPEC x-ray spectral fitting package (Arnaud 1996) which simulates both the sources found at XRCF, and the response of a flow proportional counter (FPC) or solid-state detector (SSD). It has numerous parameters which can be tuned to improve the faithfulness of the model. Some of these represent detector parameters (high voltage, electronic gain, Fano factor, etc.), while others represent source spectrum parameters (line energy, high energy cutoff for the continuum, filter thicknesses, etc.) In general most of the parameters are fixed at theoretical values and only a few are permitted to float freely during a fit to a given model. The model is discussed in Tsiang *et al.* (1997; this conference). The details of this model can be found in Tsiang (1997).

The usual XSPEC data fitting paradigm works as follows. One has a data file, consisting of a pulse height spectrum from an instrument. One has a 'response matrix', which contains within it all relevant information about the detector, including the quantum efficiency as a function of energy, and the redistribution of photons of each energy into a variety of detector pulse height channels. One then takes a theoretical model (a histogram of number of photons *vs.* energy), which can be a function of various input parameters such as temperatures, power law indices, etc., and multiplies by the response matrix (which is mathematically equivalent to the convolution of the input spectrum with the detector response). The resulting model pulse-height distribution can then be compared with the data directly. Model parameters can then be adjusted to make the model fit the data. The inverse problem (*i.e.* deconvolving the instrumental effects from the data) is in general intractable.

The present case, due to uncertainties in instrumental parameters, and to necessary adjustments needed to make the instruments perform well over an energy bandpass two orders of magnitude wide, led us to wish to be able to adjust not only source parameters during data fitting, but also detector parameters. We have therefore used a simple unit diagonal matrix for the XSPEC response matrix (telling XSPEC, in effect, that we have a perfect detector), and subsumed the convolution of the source spectrum with detector response into the source model subroutine within XSPEC. This subroutine is known as the JMKmod model, since it relies on the Jahoda & McCammon (1988) parameterization of proportional counter performance (generalized to include solid state detectors), and includes among its suite of source models narrow lines, a simple Kramer continuum of the form $(E_{\max} - E)/E$ where E is the photon energy, and a synchrotron continuum spectrum.

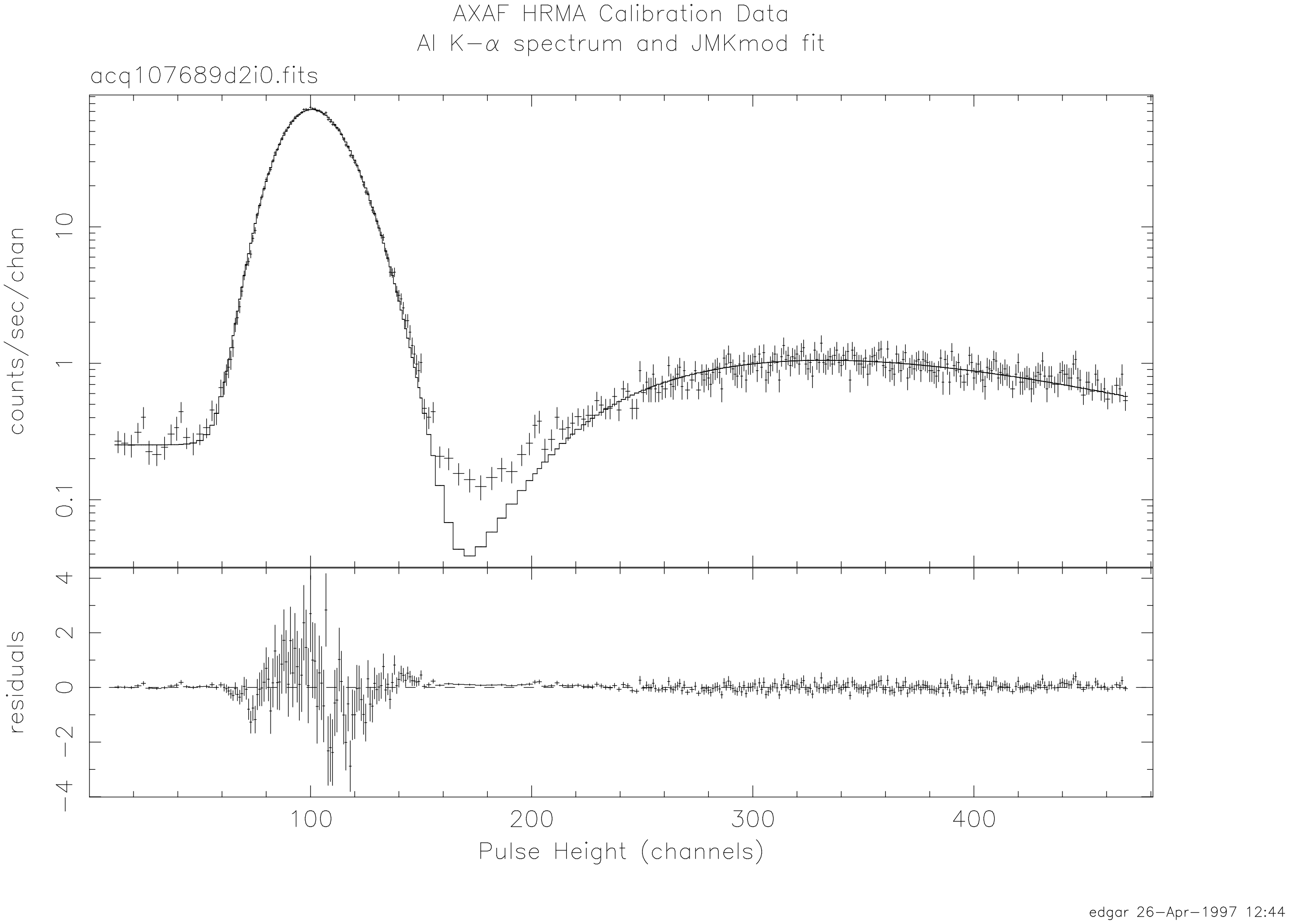

Figure 1. A typical Beam Normalization Detector Al K-α spectrum, with JMKmod fit. $\chi^2_\nu = 1.224$.

It is important to remember that the objective of the spectral fit is in most cases to recover the count rate measured by the detector in the spectral line of interest. One needs to fit the spectrum in order to understand how much of the flux in the region of interest (typically a hump in the spectrum) is due to the line, and how much may be due to continuum x-rays or background noise.

Our paradigm is that the user fits a spectrum from a detector of interest interactively using XSPEC and the JMKmod. When a satisfactory fit is obtained, and the user decides which parameters should be allowed to change from one spectrum to the next (due, for example to intensity changes, gain drifts, temperature changes, etc.), a template model is saved. This exercise is repeated for each of the detectors or detector groups (for example, the four BND-H detectors can often use the same model) of interest. Then an automated script can be run to fit all the spectra for each detector in a batch-oriented mode, and report the resulting x-ray flux at the HRMA entrance (from a weighted average of the flux of the selected BND detectors), the count rates in line and continuum for each detector, and the effective area and other quantities of interest that can be derived from the count rates. The script also obtains information contained from the HXDS "stage log", which contains the positions of all of the movable HXDS equipment at the time of each x-ray exposure (and some other times). This permits automatic identification of the aperture in use in the focal plane, and its position relative to the last-known position of the focus.

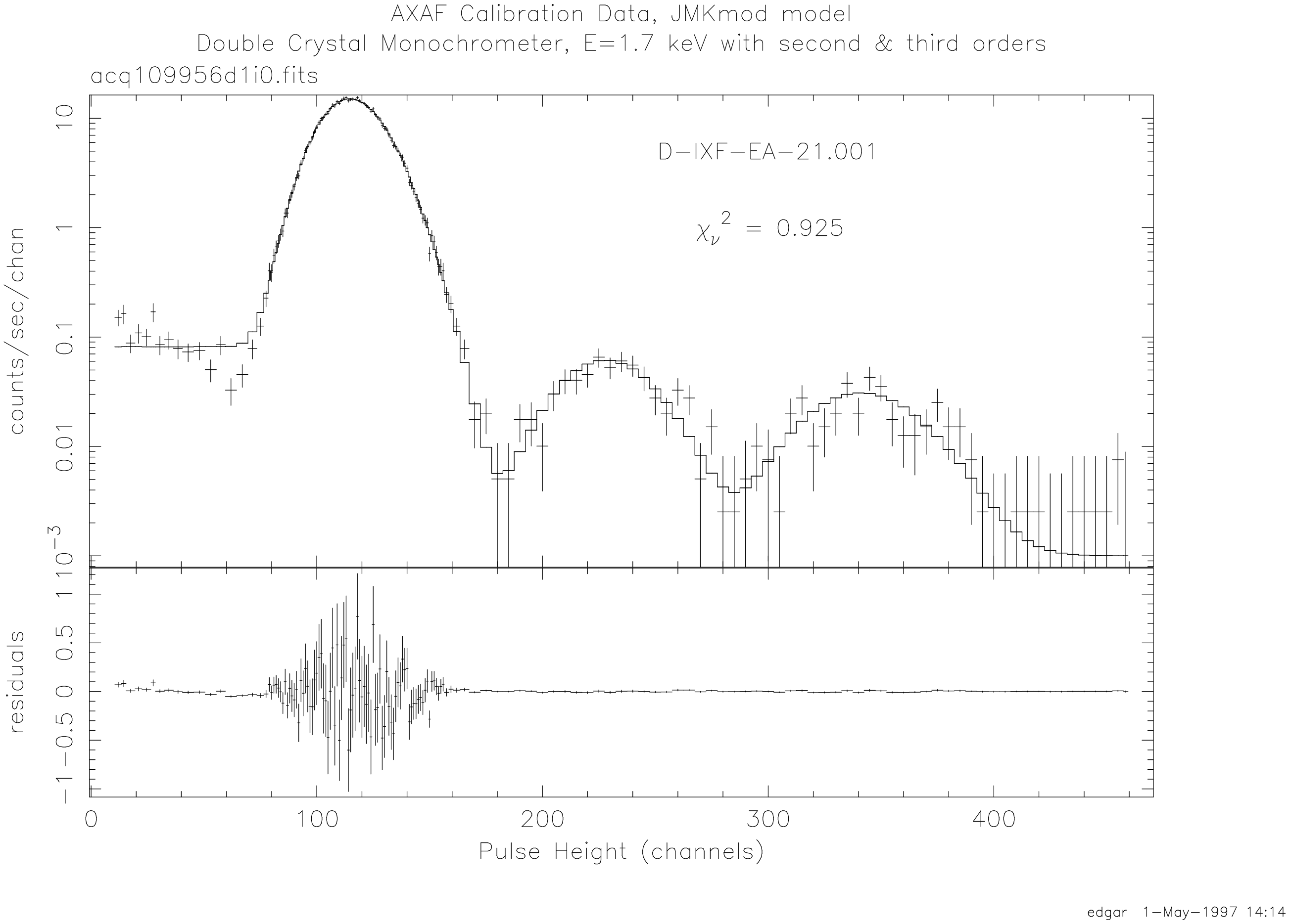

Figure 2. A Double Crystal Monochromator spectrum, with a three-line JMKmod fit.

3. FITTING PROCEDURE

We plot in Figure 1 a typical data set, and the fit we obtained, as well as the residuals from the fit. This is a spectrum produced by the Electron Impact Point Source with an aluminum anode installed, and tuned to a beam voltage of 11.88 kV. There is also a thin (17.8 μm) aluminum filter in the beam. The resulting spectrum consists of the aluminum K-α line at 1.486 keV, a continuum extending out to 11.88 keV due to Bremsstrahlung, and a large "notch" in the spectrum starting abruptly at the aluminum K-edge (1.559 keV), and getting progressively shallower towards higher energies.

The objective of this fitting procedure is to obtain the counting rate in the Al K-α spectral line. There are 53 parameters in the JMKmod model. The vast majority of these can be set to values obtained from the experiment design, the facility data (*e.g.* temperatures, maximum continuum photon energy, line energy), fixed, and forgotten. Typically the FPC gains were adjusted depending on the target line energy, to keep the line width roughly constant in pulse height bins. This also allows very low energy lines such as Be, B, and C K-α to be detected by the same detectors as high energy lines such as Fe and Cu K-α. The counter gain is a parameter of the model, which can be estimated based on the experiment setup, and then fit to the data (since it also depends on such factors as the gas temperature and pressure). The relative strengths of the line or lines and the continuum are parameters which can be frozen or fit. Finally, there are a cluster of detector parameters which govern the line shape (the Fano factor and the 'h' width parameter from the Polya function secondary electron spectrum change the width of the peak); and an

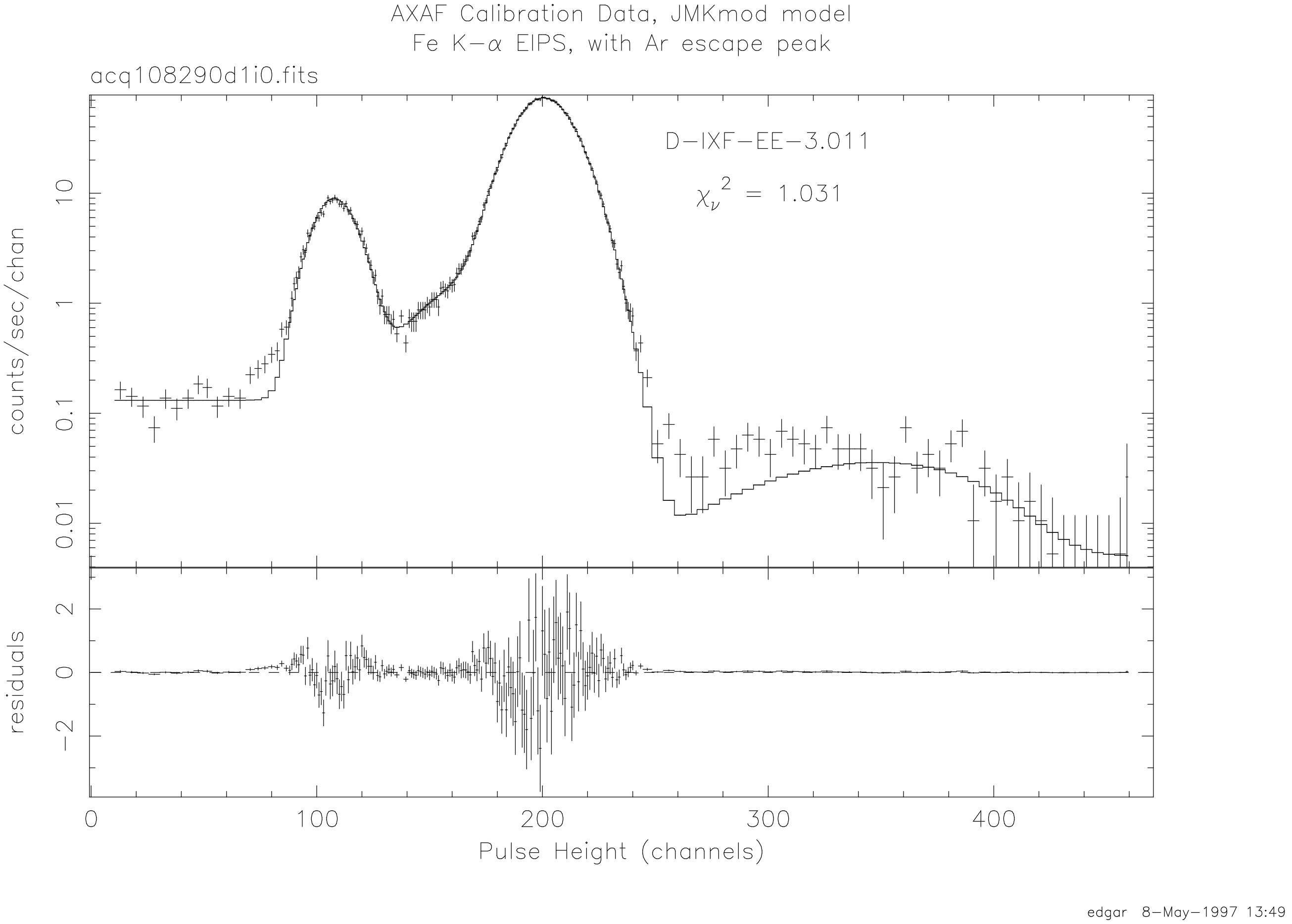

Figure 3. A typical focal plane Flow Proportional Counter Fe K-α spectrum, with JMKmod fit. $\chi^2_\nu = 1.031$.

empirical 'shelf' capability, which allows for the modeling of partial charge collection. This effect is responsible for the horizontal section of the pulse height spectrum to the left of the main peak.

We find several unexpected facility effects in the data. One is a small amount of excess flux just above the aluminum edge energy. We suspect this is due to possible pinholes in the aluminum filters. Alternatively, this may be due to unmodeled detector effects, such as argon K-α escape from continuum events above 3 keV. Another facility effect is that the high voltage we obtain by fitting the continuum spectrum often differs from the intended value by up to 10%.

In order to demonstrate the validity of the model descriptions of the line profiles, we include as figure 2 a dataset taken with the Double Crystal Monochromator, tuned to 1.7 keV. An inspection of the figure shows two higher orders, at twice and three times the advertised energy. We fit this spectrum to a JMKmod model consisting of three lines whose energies were constrained to be integral multiples of 1.7 keV. We disabled the continuum section of the code, but included the empirical "shelf," which allows for partial charge collection to be modeled. This effect manifests itself as a horizontal signal below the lowest energy peak. We also included a background, flat as a function of pulse height, at the 1.0×10^{-3} counts s^{-1}channel^{-1} level. As the figure demonstrates, the model fits nicely, with $\chi^2_\nu = 0.925$ and residuals consistent with noise.

As another example, we show in Figure 3 an iron K-α spectrum taken with the focal plane detector. X-ray photons with energies above about 12 keV are not reflected by the AXAF mirror, so we have allowed the model parameter which represents the high energy cutoff of the spectrum to float, and obtained a value of 13.4 keV (to be compared to the actual source spectrum's high energy cutoff of 36 keV before the mirror reflection).

The peak around pulse height channel 200 is the Fe K-α line, which has an energy of 6.4 keV. A manganese filter absorbs Fe K-β photons. At a pulse height of around 110 channels, the argon escape peak is visible. This peak results when 2.96 keV of energy are lost from the counter in the form of an Ar K-α photon. In this model, it is fit as a separate spectral line, with the energy constrained to be 2.96 keV less than the main peak. Also visible are a shelf, below the escape peak, a bit of continuum between the peaks, and more continuum above the manganese K edge around pulse height channel 250.

There is some tension in the fit between the continuum level at high energies and that between the main and escape peaks. When fitting beam normalization detector spectra, this effect can be quite pronounced, resulting in poor fits. We are investigating the cause of this effect, which tends to cause the model to underestimate the continuum flux above the edge. As explained below, we find that the effect of this on the measured line count rate is small.

4. IGNORED EFFECTS

There are numerous effects to be accounted for in such a fitting procedure. Here is a list of those we have done only approximately, with an estimated bias or error at the few percent level for each. They are discussed one by one below.

- The fits are done by minimizing the χ^2 statistic.
- No background subtraction is done.
- No correction is made for the mesh in the focal plane FPC window.
- Deadtime is estimated by the detector software, and we use this estimate.
- We have assumed that the quantum efficiency of all of the flow proportional counter detectors is identical.
- We assume the EIPS beam is uniform at the HRMA entrance, and estimate the flux by a straight average of the four BND-H detectors.

In cases where there are few counts per channel, the χ^2 statistic, with its built-in assumptions of Gaussian distributed errors, is both inappropriate and biased (Bevington & Robinson, 1992). A more appropriate statistic, based on maximum likelihood arguments and the Poisson distribution is discussed by Cash (1979), and Nousek and Shue (1989). This statistic is implemented within XSPEC, and only technical details of learning how to use the errors it generates prevent us from using it exclusively. We have verified that in cases with many counts per channel this C-statistic produces comparable results to the conventional χ^2 method.

For the Encircled Energy experiments, the count rates are orders of magnitude above background in every case. Therefore, for these cases, background subtraction or modeling will not be a significant effect. For wing scan spectra, since they are taken far from the core of the point spread function, and so have very low fluxes, this will be important. In those cases, because of poor statistics in the background spectra, we elected to fit a function (often a power law plus Gaussian combination) to the background spectrum, and then use this function (with no free parameters) as a component in fitting the x-ray spectra. This decision was driven in part by a feature of XSPEC which makes use of the C-statistic (see previous paragraph) incompatible with background subtraction. It also eliminates the need to deal with channels which, due to statistical fluctuations, would have a negative count rate if background subtraction were done.

The FPC detectors have a mesh of 100 micron wires on 2 mm centers to support their plastic windows against the pressure differential. For the BND detectors, which are uniformly illuminated, we have reduced the working area by the fraction of the geometrical area obscured by this mesh. For the focal plane detector, a focused, on-axis image will fit within a single mesh cell, and an effort was made to place the focused image at the center of such a mesh cell. Mesh obscuration is thought to be small in most cases. Proper accounting for this effect will ultimately be done by a ray trace.

The ratio of the quantum efficiencies of the detectors should come into the effective area. We have assumed that the detectors are identical, and so that this ratio is unity. Eventually the details of window thicknesses and counter body dimensions will need to be accounted for. We estimate this effect to be at the level of a few percent or below, except possibly at very low energies (*i.e.* the Be and B K-α lines). Ultimately the detectors will each be calibrated at BESSY, and absolute quantum efficiency calibrations will be used.

Detector dead time is estimated by the detector operating software using a Gedke-Hale technique, and we adopt this estimate (which is recorded in each raw spectral file header). An electronic pulser input was included in nearly all spectra, and a comparison of pulses injected to pulses detected will allow a more accurate dead time correction. We believe this effect is of the order of a percent.

The EIPS appears to present a beam of x-rays which is uniform at the 2% level or better at the HRMA entrance. Extensive beam mapping efforts were undertaken, and further analysis of these data is underway.

In addition, no precise facility distance numbers (*e.g.* distances from x-ray sources to detectors or the HRMA) were available at this time, so estimates were used. In most cases, errors thus introduced were less than about 0.5% for each of the effects enumerated above.

5. SENSITIVITY STUDIES

We have conducted studies to assess the effects on the target measurement (the count rate in a strong spectral line) of changes in the fitted values of other parameters in the fit. One such study was conducted by fitting data taken simultaneously by the five beam normalization FPC detectors and the beam normalization SSD. The ratios of the flux obtained were then compared to the ratio expected from simple geometric arguments, *i.e.* presuming the beam is uniform, the ratio is just the ratio of aperture areas over the ratio of the squares of the source distances. Account must also be taken for the 90.25% transmission of the window support mesh in the FPCs. When this is done, we find agreement to within 2% at Al K-α. The agreement is somewhat worse at low energies (such as B and C K-α), and at high energies (Fe K-α and above). This is probably a real effect, namely a difference in the quantum efficiency (QE) among the BND detectors. We look forward to synchrotron calibrations of the detectors, in which the QE of each detector will be measured at a variety of energies.

Another fitting effect that potentially impacts the accuracy of the line count rate in the focal plane detectors is that the mirror reflectivity is a function of photon energy. In those cases where the continuum high-energy cutoff is above that of the mirror, we typically allow the model parameter that represents this cutoff energy to float during the fit, and settle to a fictitious lower value, in order to fit the (mirror modified) continuum. Satisfactory fits can be obtained in most cases in this manner. When the actual mirror effective area is known, a “filter” can be inserted into the model, which will modify the spectrum accordingly, and this practice will no longer be required.

In order to assess the effects of this lowering of the continuum high energy cutoff, we obtained line counting rates for various fixed values of the high energy continuum cutoff parameter. We find that, while the reduced χ^2 is substantially worse for the “wrong” value of this parameter, the fitted value of the line counting rate remains the same, to within 0.7%.

We also find that either of the line width parameters for the FPC fits, the Fano factor and the Polya h parameter, can be used to fit the line width, with comparable results both in terms of χ^2 and the fitted line counting rate. In this case, the counting rate is the same to within 0.03%.

These studies were conducted with high signal-to-noise ratio spectra, generally at the C and Al K-α lines, so as to assess the effects of model parameters on the line count rate, in the absence of confusion generated by poor statistics.

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6. REFERENCES

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Arnaud, K.A., 1996, *Astronomical Data Analysis Software and Systems V*, eds. Jacoby G. and Barnes J., p17, ASP Conf. Series volume 101.

Bevington, P. R., & Robinson, D. K. 1992, *Data Reduction and Error Analysis for the Physical Sciences* (New York: McGraw Hill).

Cash, W. 1979, ApJ, 228, 939.

Jahoda, K., and McCammon, D, 1988, Nuclear Instr. and Methods, A272, 800.

Tsiang, E. Y. *et al.* 1997, this conference.

Tsiang, E. Y. 1997, JMKmod User Manual, publication SAO-AXAF-DR-97-276.