Chapter 4

Measurement of the Sub-pixel Structure of Chandra CCDs

4.1 Introduction

As already discussed, the ambitious scientific objectives of Chandra require precise knowledge of the instrumental response, i.e. energy scale, spectral resolution and detection efficiency. For example, the calibration goal for the quantum efficiency (QE) of the ACIS detectors is 1% accuracy (Weisskopf et al. 1995). In §3.6.1, we found that the most accurate model of the low energy detection efficiency requires determination of the dimensions of the sub-pixel structures (i.e. the channel stops and each of three gates). At sufficiently low energies ($E \lesssim 4.0$ keV), the characteristic absorption length of X-rays is sufficiently smaller than the depletion depth (between 60 and 70 $\mu$m for ACIS devices) that the expression for QE reduces to:

$$QE(E) = \left(\prod_{\text{gate}} e^{-(d/\lambda(E))}\right) \left(1 - w\right) + w \left[\prod_{\text{CS}} e^{-(d/\lambda(E))}\right],$$

(4.1)

where the three terms in the gate product represent absorption by layers of Si, SiO$_2$, and Si$_3$N$_4$ and the two terms in the second product represents absorption by the $p^+$-type Si and SiO$_2$ that comprise the channel stop, which covers a fractional area.
In Chapter 3, I showed that broad-band synchrotron data give excellent constraints on the three gate parameters for the QE model, provided that all other relevant parameters are frozen. In general, these data cannot uniquely constrain all six parameters in Equation 4.1. Among the most significant of the degeneracies is that between the overall width of the channel stops, on the one hand, and the thickness of the gate structure, on the other hand. This ambiguity in gate structure parameter values can lead to large errors in the estimated detection efficiency, particularly near the characteristic absorption edges where the gate opacity can be large.

The measurements reported in this Chapter were made to improve the ACIS calibration accuracy by resolving some of these ambiguities. In particular, I discuss one approach for the measuring the channel stop structure, represented by a model with five parameters. This technique also provides constraints on the dimensions of the three different polysilicon and SiO$_2$ layers that comprise the actual gate structure. Our method also shows a correlation between event grade and location of the event interaction within a pixel, information that has the promise of yielding sub-pixel spatial resolution.

Closer examination of our preliminary results revealed inconsistencies between some of the measurements. Specifically, the thickness of the channel stop oxide and p$^+$-type silicon determined from measurements at low and high energies did not agree. We began investigating the nature of charge collection in the channel stop region and discovered that the amount of charge collected from an event interacting in the p$^+$-type silicon depends on the voltage applied to the gate directly above the channel stop. These results are discussed in §4.8.

While the sub-pixel structure is clearly visible in the preliminary data, higher resolution would allow more accurate measurements and significantly reduce the the rather complicated analysis. Armed with our better understanding of the physics of charge collection in the channel stop region, we modified our experimental technique to significantly improve the quality of our sub-pixel measurements. In §4.9, I
discuss these improved data and present a self-consistent model that allows accurate determination of the thicknesses of the channel stop materials.

4.2 Experimental Method

4.2.1 Concept

We used a metal foil with regularly spaced holes (hereafter, mesh) to illuminate the CCD with very narrow beams of monochromatic X-rays and observe the dependence of the detector response on the location of photon interaction inside the pixel. When the mesh is placed close to the CCD surface and rotated with respect to the axes defined by the gate structure and channel stops, a moiré pattern is formed when the device-mesh combination is illuminated with X-rays. This technique was first used with CCD detectors by Tsunemi et al. (1997). Changes in relative count rates reflect attenuation of the incident flux by the dead layers of the sub-pixel structure. By repeating the measurements at a number of X-ray energies, specifically energies above and below both the Si Kα and O Kα absorption edges, the widths and thicknesses of the gates, channel stops, and insulators can be uniquely determined.

The mesh used in our first experiments consists of a 10 μm thick copper foil with a square array of 4 μm diameter holes spaced every 24 μm. Refer to Figure 4-1 (left) to see a section of the mesh and its orientation to the CCD. For the range of X-ray energies used, the mesh has a maximum transmission of $6.0 \times 10^{-3}$, but typical transmissions are generally below $7.0 \times 10^{-5}$. The mesh was stretched taught to remove wrinkles and was held parallel to the surface of the CCD to keep the illumination pattern circular and uniform. It also needs to be as close to the CCD as possible to minimize the broadening of the point spread function (PSF) due to finite beam divergence and diffraction effects. To meet all three requirements, we fabricated a special fixture to hold the mesh. Figure 4-1 shows a cross section of this holder.
4.2.2 Moiré Phenomena

The mesh holes have a nominal periodicity of 24 μm, corresponding to the pitch of the ACIS CCD pixels. Smaller spacings would result in two different holes illuminating the same pixel and would mix the spatially dependent response of the pixel. At the same time, the mesh must be rotated with respect to the axes defined by gates and channel stops to ensure an equal and complete mapping of the pixel’s response to the incident photons. The resulting data can be understood in the context of a moiré pattern.

The details of the moiré phenomena are presented in Appendix B. For a mesh with periodicity $D'$, not equal to the CCD pixel pitch $D \equiv 24 \mu m$, rotated an angle $\theta$ with respect to the CCD, the angle $\varphi$ the moiré pattern makes with respect to the CCD is given by:

$$\varphi = \frac{\pi}{2} - \theta + \tan^{-1}\left(\frac{1 - \epsilon \cos(\theta)}{\epsilon \sin(\theta)}\right) ; \; \epsilon \equiv \frac{D'}{D} \quad (4.2)$$

Typically, the mesh was rotated about one degree with respect to the CCD. The values of $\varphi$ observed were on order of five degrees, indicating that the mesh spacing $D'$ is not equal to 24 μm. Given the tolerances used in the mesh fabrication and the possibility of deformation due to thermal and mechanical stresses, the deviation of the periodicity from 24 μm is not unexpected. The dimension of the spacing does not
affect the results, as long as it stays constant during the course of the experiment.

4.2.3 Data Acquisition

After the mesh holder was fixed to the CCD housing, the CCD-mesh assembly was placed in a vacuum chamber and cooled down to the standard operating temperature of \(-120^\circ\) C. Two different systems were used to produce the monochromatic X-ray beam. A grating monochromator and electron impact source (IFM) produced photons corresponding to the O K\(\alpha\) line (525 eV) and a photon fluorescence source (HEXS; Jones et al. 1996) was used to excite the K\(\alpha\) lines of Al, Si, P, Cl and K. The use of the specialized holder illustrated in Figure 4-1 (right) kept the mesh taught and parallel and placed it within 200 \(\mu\)m of the surface of the CCD, the closest distance achievable while preventing the risk of damage to the flight quality CCD from accidental contact with the mesh. The gap, however, effectively increased the diameter of the mesh holes by geometric shadowing. To reduce this effect, the divergence of the incident beam was minimized by using an aperture and placing the CCD as far away from the source as possible, while maintaining an acceptable incident flux rate. Baffles were also used to prevent specular reflection from widening the beam pattern. Figure 4-2 shows the experimental set-up. Given the location of the X-ray source, the CCD and the nominal 4 \(\mu\)m diameter of the holes, the X-rays cast an image of diameter 4.2 \(\mu\)m on the CCD. The large distance between the CCD and X-ray source and the small open area of the mesh (2.8%), required significant time to accumulate statistically significant data. Table 4-1 summarizes all the data acquired, including which X-ray source was used, the photon energy and the corresponding K\(\alpha\) emission line, the number of distinct measurements, the total integration time, and total number of events in the monochromatic line.
Figure 4-2 View of the experimental setup use for initial mesh measurements. The IFM and HEXS X-ray sources have their own beam lines and use different vacuum vessels to house the CCDs, but the same apertures were used and placed at the same distances in both cases. Dimensions are in inches, unless otherwise noted.

Table 4-1: Summary of initial mesh measurements.

<table>
<thead>
<tr>
<th>X-ray Source</th>
<th>$Kα$</th>
<th>Energy (eV)</th>
<th>Data Sets</th>
<th>Time (hour)</th>
<th>Total Events</th>
</tr>
</thead>
<tbody>
<tr>
<td>IFM</td>
<td>O</td>
<td>525</td>
<td>3</td>
<td>8</td>
<td>$6.1 \times 10^5$</td>
</tr>
<tr>
<td>HEXS</td>
<td>Al</td>
<td>1487</td>
<td>4</td>
<td>98</td>
<td>$1.8 \times 10^5$</td>
</tr>
<tr>
<td>HEXS</td>
<td>Si</td>
<td>1740</td>
<td>4</td>
<td>129</td>
<td>$2.4 \times 10^5$</td>
</tr>
<tr>
<td>HEXS</td>
<td>P</td>
<td>2015</td>
<td>5</td>
<td>91</td>
<td>$4.4 \times 10^5$</td>
</tr>
<tr>
<td>HEXS</td>
<td>Cl</td>
<td>2622</td>
<td>2</td>
<td>81</td>
<td>$1.3 \times 10^5$</td>
</tr>
<tr>
<td>HEXS</td>
<td>K</td>
<td>3312</td>
<td>2</td>
<td>81</td>
<td>$4.7 \times 10^5$</td>
</tr>
</tbody>
</table>

### 4.3 Data Analysis and Results

Analysis begins by performing a bias correction on each of the raw CCD images and extracting the events that lie in the photo-peak of the monochromatic line. We then
filter the data by selecting suitable event grades, single pixel (grade 0), horizontally split events (grades 3 and 4), vertically split events (grade 2), and corner events (grade 6), and create the fundamental moiré pattern for each types. Each fundamental pattern consists of a collection of smaller moiré cells which reveals the pixel’s spatial response to the photons. These individual moiré cells must be rotated before the data can be summed together to form one representative pixel (hereafter RP) for the entire CCD. Due to uncertainties in the mesh rotation angle $\theta$ and the mesh periodicity $D'$, we do not rely on Equation 4.2 to calculate the rotation angle $\varphi$, but rather determine it from the data using essentially a Fourier technique. The left panel of Figure 4-3 shows a sample of the raw, unrotated moiré pattern (O K\(\alpha\), grade 0) that is a direct output of the illumination of the mesh-CCD system. The right panel of Figure 4-3 repeats the RP in a $3 \times 3$ array to make it easy to see the boundary regions of the pixel.

Figure 4-3 Raw and deconvolved moiré data. *Left:* The fundamental moiré pattern for single pixel (grade 0) events at O K\(\alpha\) (525 eV). The individual moiré cells are clearly discernible. *Right:* The representative pixel (RP) repeated in a $3 \times 3$ array. The vertical stripe in the fundamental image is a quadrant boundary in the CCD detection algorithm.

Figure 4-4 displays a grid of $3 \times 3$ RP arrays for grade 0, grade 2, grades 3 and 4, and grade 6 events for three of the six K\(\alpha\) line energies (O K\(\alpha\), Cl K\(\alpha\), and Si K\(\alpha\)). Each column has the same energy, and each row has the same grade. The
characteristic absorption length increases from left to right. The confinement of event grades to particular regions of the pixel (i.e. grade 2 events only occur along the vertical boundaries of the pixel) offers conclusive, experimental proof that event grades have physical significance that corresponds to photons that interact in the center, the edges or the corners of the pixel. This information is explored further in Section 4.7 when the possibilities of obtaining sub-pixel resolution are explored. The figures also contain graphs of the count rates for the RP summed in the direction parallel to the channel stops (the horizontal graphs) and the direction parallel to the gates (the vertical graphs). These one dimensional rate plots clearly show the attenuating effects of the sub-pixel structures, and it is analysis of these data that provides information about the channel stops and gates.

4.4 Determination of the Channel Stop Dimensions

Conceptually, the approach for determining the channel stop dimensions is very direct. The deficiency of detected photons predicted by a model of the channel stop is convolved with the PSF of the mesh holes. The resultant convolution is compared to the experimental data, and the channel stop model parameters are allowed to vary, using a $\chi^2$ fit statistic to determine the best fit parameters.

Channel stops are fabricated using a standard LOCOS technology (Burke et al. 1994), where a portion of the Si$_3$N$_4$ insulating layer is etched away and boron is implanted in the opening, forming a strip of p$^+$-type silicon. Then the silicon is oxidized, thickening the insulating layer of SiO$_2$ directly above the implanted stop. Figure 4-5 is an SEM measurement of a CCD cleaved to expose the channel stop. The black and white bands at the top of the image are the polysilicon gates and insulating oxide, respectively. The elongated, hexagonal structure is the SiO$_2$ insulator between the p$^+$ region (not visible in this image) and the gates. The thin white structure between the gates and hexagonal insulator is the Si$_3$N$_4$. The p-p$^+$ transition cannot
Figure 4-4 3 × 3 arrays of grade 0, grade 2, grades 3 and 4, and grade 6 Representative Pixels (RP). Each column has the same energy, and each row has the same grade. The data are presented in order of increasing silicon attenuation length: O Kα (left), Cl Kα (middle), and Si Kα (right).
be seen in this photograph. We adopt a five parameter model to represent the channel stop. Figure 4-6 shows the five parameter channel stop model we adopt in our fitting.

Figure 4-5 SEM photograph of an ACIS CCD cleaved to show the channel stop structure. The broad black and white bands near the top of the image are the polysilicon gate and insulating layer of SiO$_2$, respectively. The elongated, hexagonal structure is the SiO$_2$ insulator between the p$^+$ region (not visible in this image) and the gate structures. The thin white structure between the gates and hexagonal insulator is the Si$_3$N$_4$. The bar is 1.0 $\mu$m.

![Figure 4-5 SEM photograph of an ACIS CCD cleaved to show the channel stop structure.](image)

Figure 4-6 The five parameter model used in determining the dimensions of the channel stop.

In addition to constructing a realistic channel stop model, the success of this technique depends on use of an accurate PSF for the mesh and accounting for additional processes that effectively broaden the PSF (i.e. diffraction, diffusion of the charge...
cloud, distortions to the PSF caused by using a non-parallel X-ray beam). Computing such an aperture function (hereafter AF) analytically is a daunting task. Fortunately, the AF can be ascertained from the mesh data itself. Horizontal and vertical split events come from photons that interact within an electron cloud size diameter of the pixel boundary. The spatial distribution of vertical split events ($\Delta v_{\text{split}}$) is given by the convolution ($\otimes$) of three terms:

$$\Delta v_{\text{split}} = PSF \otimes C_i \otimes D,$$

(4.3)

where PSF is the point spread function of the mesh hole, $C_i$ is the initial charge cloud size\textsuperscript{1}, and $D$ is a term that describes how the initial charge cloud diffuses as the cloud moves under the influence of the electric field created by the potential applied to the gates. The amount the initial charge cloud diffuses varies dramatically with energy, so we use an unique AF for data taken at each energy. The number of detected events ($N_{\text{detected}}$) is given by:

$$N_{\text{detected}} = PSF \otimes C_i \otimes D \otimes M_{CS},$$

(4.4)

where PSF, $C_i$, and $D$ are the same as above and $M_{CS}$ is the model of the channel stop. If we define the AF as the ($\Delta v_{\text{split}}$)

$$AF \equiv \Delta v_{\text{split}} = PSF \otimes C_i \otimes D,$$

(4.5)

Equation 4.4 simply becomes

$$N_{\text{detected}} = AF \otimes M_{CS}.$$

(4.6)

The data presented in Figure 4-7 shows the relative amount of attenuation caused

\textsuperscript{1}Analysis of double crystal monochromator data performed by Prigozhin et al. (2000) indicate that the initial cloud sizes range between 10 and 100 nm.
by the channel stops. The amount of attenuation is governed entirely by the characteristic attenuation lengths of the Kα photons in Si, SiO₂, and Si₃N₄ and therefore does not simply monotonically increase with increasing photon energy.

![Attenuation due to the Channel Stop](image)

**Figure 4-7** Variation in detection efficiency due to differing amounts of attenuation in the dead layers of the channel stop.

Fitting the channel stop model to data from only one energy results in degeneracies in the best fit parameters. To constrain these parameters, we perform a simultaneous fit of several data sets taken at different energies. The upper two panels of Figure 4-8 show the χ² confidence plots for the O Kα data set and the P Kα data sets. The contours are for the 68%, 90% and 99% confidence levels. The box and wing parameters have large uncertainty, but the constant slope of the contours does indicate a bound to the total width. The situation is similar for the thicknesses of the Si p⁺ layer and the insulating SiO₂. By simultaneously fitting multiple data sets, a tighter constraint can be placed on the model. The bottom panels of figure 4-8 show the χ² contours for the five HEXS data sets (Al, Si, P, Cl, and K). Taken together, these data provide a good measure of the width parameters and the p⁺ and SiO₂ thicknesses. Table 4-2 lists the parameter, the range of parameter space and grid size used, and
the derived best fit-value (90% confidence level) from the simultaneous fitting.

Comparing the O Kα χ² contours with the combined HEXS data χ² contours in Figure 4-8 reveals that the data taken with the two different X-ray sources do not completely agree. This difference is shown in Figure 4-9, which plots the predicted attenuation, based on the HEXS best fit parameters, and the data for all six energies. The models work well for all but the O Kα data.

At the time of these experiments, the best explanation for the degeneracy was the use of an overly simplistic model that did not properly account for all the relevant physics. Key to our model was the assumption that the gate structures and channel stops are dead layers. However, it was known that this is not entirely correct. Prigozhin et al. (2000) have explained the origin the low energy tail of the spectral redistribution function as being associated with low-penetrating X-ray events. They show that when a photon interacts near the gate oxide or nitride, only a fraction of the charge is collected. We speculated that similar processes may occur for photons that land close to the SiO₂ region of the channel stop.

A larger uncertainty was the exact physical process that occurs in the doped p⁺ stop. The dopant concentration decreases non-linearly as a function of distance from the insulating oxide layer. It seemed plausible that the charge from photons interacting in the lower p⁺ concentration regions is fully collected. Another possibility was that the charge from X-rays interacting in a region of moderate p⁺ concentration

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Table 4-2: Channel stop values derived from HEXS data

<table>
<thead>
<tr>
<th>Name</th>
<th>Search range</th>
<th>Step size</th>
<th>Best-fit value</th>
</tr>
</thead>
<tbody>
<tr>
<td>box width</td>
<td>3.1 − 4.5 µm</td>
<td>.16 µm</td>
<td>4.2⁻²⁺.4 µm</td>
</tr>
<tr>
<td>wing width</td>
<td>0.12 − 1.2 µm</td>
<td>.12 µm</td>
<td>.35⁻¹⁺.12 µm</td>
</tr>
<tr>
<td>Si thickness</td>
<td>0.12 − 1.2 µm</td>
<td>.12 µm</td>
<td>.35⁻⁶⁺.06 µm</td>
</tr>
<tr>
<td>SiO₂ thickness</td>
<td>0.12 − 1.2 µm</td>
<td>.12 µm</td>
<td>.71⁻¹⁺.17 µm</td>
</tr>
<tr>
<td>Si₃N₄ thickness</td>
<td>0.0 − 0.05 µm</td>
<td>.01 µm</td>
<td>insensitive</td>
</tr>
</tbody>
</table>
Figure 4-8 $\chi^2$ contour plots for box width vs. wing width and Si p$^+$ depth vs. SiO$_2$ depth. Contours are the 68 %, 90 %, and 99 % confidence levels. The top row is for the O K$\alpha$ data, the middle row for the P K$\alpha$ data, and the bottom row for the simultaneous fit of all five HEXS measurements.
might only be partially collected. If these effects were real, we speculated that incorporating them into our model would improve the detection efficiency beneath the channel stop, particularly at low energies. This increase in detection efficiency at O Kα energies would lead to better agreement between data and theory.

In fact, we have shown that incomplete charge collection is the relevant process for events interacting in the channel stops. In Chapter 5, I explain the experiments undertaken to study and explain this phenomena. As I show in §4.9, this effect must be accounted to properly interpret the mesh data.

Figure 4-9 Best-fit HEXS channel stop model compared to experimental data.
4.5 Determination of the Gate Structure Dimensions

The determination of the gate structure dimensions follows a method analogous to that used in the channel stop analysis. The single event and vertically split RPs are added together and summed in the direction parallel to the gates, excluding the corner and horizontal regions of the RP where grade 6 and grade 3 and 4 events occur. A model of the gates is convolved with the same AF used for the channel stops (refer to Section 4.4), the convolution is compared to the data, and the model is adjusted until $\chi^2$ is minimized.

After the channel stops are implanted in the bulk silicon, the gates are formed using a triple-polysilicon process (Burke et al. 1994). A layer of polysilicon is deposited on the $\text{Si}_3\text{N}_4$-$\text{SiO}_2$ dielectric layer that covers the bulk silicon. Roughly two-thirds of the polysilicon is etched away in a piece-wise, periodic fashion (i.e. 16 $\mu$m of every 24 $\mu$m is removed), and the remaining strips are oxidized, creating a protective layer of $\text{SiO}_2$ over the first gate ($\phi_1$). The entire deposition-etching-oxidation process is repeated twice more to form the second and third gates ($\phi_2$ and $\phi_3$, respectively). Figure 4-10 is a SEM measurement made on a CCD cleaved to expose the gate structure. The black and white structures towards the top of the image are the polysilicon gates and insulating $\text{SiO}_2$ layers, respectively. The upper, parallel band running across the middle of the image is a dielectric layer of $\text{Si}_3\text{N}_4$, and the lower, parallel band is a dielectric layer of $\text{SiO}_2$. The bulk silicon on which these structures are grown is not visible in this image. This particular photograph shows the overlap between a $\phi_2$ and $\phi_1$ gate. Figure 4-11 shows the fifteen parameter model used to represent the gate structure. In our fitting we fix the thickness of the uniform nitride and oxide layers that run between the polysilicon gates and bulk silicon. We further simplify the model by not including the small width (less than 0.2 $\mu$m in the SEM
photographs) of insulating SiO$_2$ that occurs between gates.

Figure 4-10 SEM photograph of a CCD cleaved to expose the gate structure. The white structure closest to the top of the image is the insulating SiO$_2$ layers grown on top of the polysilicon gates, the two black structures (the flat one on the left side and the reverse sigmoidal one on the right side of the photos). The upper, parallel band running across the middle of the image is the Si$_3$N$_4$ layer and the lower, parallel band is another SiO$_2$ layer. The bulk silicon on which these structures are grown is not visible in this image. The bar in the photo is 1.0 $\mu$m. This particular photograph shows the overlap of a $\varphi_2$ gate (the reverse-sigmoidal black structure) on a $\varphi_1$ gate.

Figure 4-11 The fifteen parameter model used to describe the gate structure.
Figure 4-12 compares the best fit model with the raw the O Kα data. The best fit parameters are printed in the upper right. The dashed line shows the efficiency predicted by the model and normalized to previously determined quantum efficiencies. Qualitatively, the model fits the data quite well and produces reasonable parameter values, i.e. they are consistent with the dimensions determined by SEM measurements similar to Figure 4-10. Unfortunately, the number of free parameters in the model produces results in large uncertainties in the best fit parameters. When determining the structure of the channel stops, we relied on multiple data sets to break the degeneracy in the model. In the case of the gate structure, however, only the O Kα data shows statistically significant variation in detection efficiency. For the five data sets taken at other energies, the characteristic absorption lengths in Si and SiO₂ are much larger than the thickness of the polysilicon and oxide layers. The relative thinness of the gates (compared the attenuation lengths) results in nearly uniform attenuation across the pixel and prevents a further refinement in the parameter values determined from the O Kα data.

While the current data do not provide the exact dimensions of all the layers that comprise the gate structure, it does provide some useful constraints. The different quantum efficiencies under each of the gates clearly indicates that the polysilicon and SiO₂ layers that comprise φ₃ are thinner than the layers that comprise φ₂, which in turn are thinner than the layers that comprise φ₁. The shape of the three, broad curves in the data give some measure of the width of each of the gates. Additional information, either from design specifications (the total width of all three gates cannot exceed 24 μm) or independent measurements (e.g., SEM studies or the CCD’s response to undispersed synchrotron radiation [Chapter 3]), provides further constraints on the dimensions of the gate structure.
Figure 4-12 Quantum efficiency across the gate structure, best fit model with the data at O Kα. The best fit parameters appear in the upper left of the plot. The dotted line shows the predicted attenuation due to the absorption of photons in the dead layers of the gate. Refer to Figure 4-11 for the physical structure of gates $\phi_1$, $\phi_2$, and $\phi_3$. 
4.6 Additional Results

4.6.1 Clocking Effects

In addition to acting as a probe for the sub-pixel architecture, the mesh-moiré experiments nicely illustrate the effects of different gate bias schemes. Typically, gates $\phi_2$ and $\phi_3$ are held high and gate $\phi_1$ is held low (refer to Figure 4-11 for gate definitions.) This configuration places the vertical potential energy maximum, and hence the vertical pixel boundary, in the middle of $\phi_1$. Thus, the peak location for grade 2 events should correspond to the middle of $\phi_1$. Figure 4-13 plots the quantum efficiency across the pixel. Again, the dashed line shows the model gate structure. The dotted line shows the grade 2 contribution to the total quantum efficiency. The location of the peak beneath $\phi_1$ is additional proof that grade 2 events result from photoabsorptions that occur close to the vertical boundary of a pixel.

Figure 4-13 Quantum efficiency across the gate structure for O K$\alpha$. The hashed line shows the data, the solid line shows the model (the sum of grade 0 and grade 2 events), and the dotted line shows the location and contribution of the grade 2 events. Clocking scheme: $\phi_1$ low, $\phi_2$ and $\phi_3$ high.
When the bias on either $\phi_2$ or $\phi_3$ is switched to the low state\(^2\), the location of the grade 2 distribution peak should shift to the new location of the vertical potential energy maximum. To first order, when only $\phi_2$ is held high, the grade 2 peak should shift to the region between $\phi_1$ and $\phi_3$ (refer to Figure 4-14 [top]). To first order, when only $\phi_3$ is held high, the grade 2 peak should shift to the region between $\phi_1$ and $\phi_2$ (refer to Figure 4-14 [bottom]). In both of these cases, the exact location of the grade 2 peak is influenced by the differing thicknesses and widths of the polysilicon gates and insulators, and deviations from the first order predictions are expected.

Physically, the device does not change so the low energy quantum efficiency of the CCD remains constant, independent of the particular bias configuration. At the same time, the branching ratios of grade 2 (g2) events, and correspondingly, grade 0 (g0) events\(^3\) are clearly influenced by the bias scheme. Ideally, all events would be single pixel events to maximize the energy resolution performance of the CCD.\(^4\) A judicious choice of bias schemes ($\phi_2$ and $\phi_3$ high, $\phi_1$ low) guarantees that the location of the vertical pixel boundary will occur under the least efficient portion of the detector, and hence, guarantees the highest grade 0 branching ratio.

### 4.6.2 Evidence of Charge Cloud Diffusion

The mesh-moiré experiments also give insight into the role diffusion plays in the increase in the size of the charge cloud. After the initial photoelectric absorption and creation of the charge cloud by secondary electrons, the cloud drifts upward towards the gates under the influence of the electric field in the depletion region. Although the fields are strong and diffusion times are small, the cloud does expand radially. This process can again be seen by examination of the vertical split events.

\(^2\)At least one gate must be high to create the potential minimum needed to define a vertical boundary between pixels.

\(^3\)The sum of the g0 and g2 branching ratios must be constant for the overall detection efficiency to be constant.

\(^4\)Every pixel has a $\sigma_{\text{noise}}$ term associated with it. When summing charge from multiple pixels, the $\sigma_{\text{noise}}$ terms get added in quadrature.
Figure 4-14 Quantum efficiency across the gate structure for O Kα. The hashed line shows the data, the solid line shows the model (the sum of grade 0 and grade 2 events), and the dotted line shows the location and contribution of the grade 2 events. 

*top:* Clocking scheme: $\phi_1$ and $\phi_3$ low, $\phi_2$ high. 

*bottom:* Clocking scheme: $\phi_1$ and $\phi_2$ low, $\phi_3$ high.
Figure 4-15 contains the widths (FWHM) from a Gaussian+constant fit to the grade 2 distributions.

**Figure 4-15** Attenuation length and charge distribution width as a function of energy

*Top:* the Gaussian FWHM of the grade 2 events as a function of attenuation length of the incident photons. *Bottom:* the Gaussian FHWM of the grade 2 events (right axis) and the attenuation length (left axis) as a function of photon energy. The solid line is the attenuation length, the discrete points are the measured widths. Errors on the FWHM values are much smaller than the symbols used.

The distributions are the convolution of the mesh PSF with the charge cloud after it has diffused to the potential energy minimum. In fact, this convolution of mesh PSF, initial charge cloud size, and diffusion effects is the AF defined in Equation 4.5. As the PSF and initial charge cloud size are largely independent of energy, the widths provide a way to study the effects of diffusion. The upper panel plots the FWHM vs. attenuation depth in Si and shows the expected trend that the widths increase with increasing attenuation length. The lower panel plots both the FHWM (left
axis) and the Si attenuation length (right axis) vs. energy. The data indicate that
the width of the distribution is not a monotonically increasing function of energy.
To quantitatively model the diffusion process requires both a 2-D simulation of the
electric potentials as well a model of the charge distribution within the initial cloud
and is beyond the scope of this paper. However, data of this nature will certainly
help such efforts.

4.7 Prospects for Sub-pixel Resolution

In addition to revealing the dimensions of the sub-pixel structure, this technique
provides information that may be useful in improving the spatial resolution of the
CCD beyond that of a 24 µm × 24 µm pixel device. The origin of different event
grades has long been considered to depend on the location of the photon interaction
within a pixel (e.g., Janesick, Elliott, & Garmire 1985 and Bautz et al. 1987), and
these mesh experiments conclusively prove that supposition. These mesh experiments
conclusively prove that the event grade is dependent on the location of the photon
interaction within a pixel. Referring to the plots of the RP arrays in Figure 4-4, it
is clear that grade 0 events come from photons landing in the pixel center, grade 2
events come from photons landing close to the vertical pixel boundaries, while grade
3 and 4 events come from photons landing near the horizontal pixel boundaries, and
grade 6 events come from photons landing in the pixel corners.

The confinement of certain event grades to a specific area of the CCD is effectively
like having smaller pixels inside a 24 µm pixel and is the key to obtaining sub-
pixel resolution. The ratio of single pixel events to multiple pixel events is a strong
function of energy and penetration depth of the photon into Si. As the percentage
of multiple pixel events increase, these mini-pixels will increase in size. Figure 4-
16 shows two 3 × 3 pixel grids. Both grids show a geometric area (computed from
the branching ratios) for the different event grades discussed above, one for Si Kα
photons (1.740 keV) and one for Cu Kα photons (8.040 keV). Superimposed on each

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Figure 4-16 Chandra HRMA encircled energy surfaces projected onto a schematic of sub-pixel locations.
of these grids are the 33 % and 66 % enclosed energy curves for the Chandra HRMA. A full, mathematical investigation has not been performed, but the hope is that by comparing the branching ratios from an astronomical observation with ground calibration data, the source location can be determined to better than one pixel.

4.8 Charge Loss in the Channel Stops

Channel stops occupy a noticeable fraction of a CCD pixel. At low energies, a significant fraction of photon interactions will occur in the vicinity of the oxide and p+ implant and have a noticeable effect on the redistribution function. We have performed a series of experiments to study and understand these important processes. I explain these measurements in great detail in Chapter 5. Here, I summarize the results germane to the mesh experiments.

The region inside the doped p+ silicon is effectively field free. Any photon interacting there creates an electron cloud which spreads out in all directions due to diffusion. Some fraction of the cloud will reach the surface and recombine, if there is a potential well for the electrons at the Si-SiO$_2$ interface due to a positive gate voltage. In this case, not all the charge will be collected. If the gate voltage is negative, electrons are reflected back into silicon and eventually get collected into the CCD potential well in the buried channel. In this case electron cloud does not suffer any charge loss. Those events landing in the channel stop beneath a negatively biased gate will contribute to the main, Gaussian-shaped photopeak, while those landing beneath a positively biased gate will contribute to the “shoulder,” a tail extending to the low-energy side of the main peak.

The dramatic influence the gate voltage has is vividly seen in the mesh data. Figure 4-17 (top) shows a spectral redistribution function for for monochromatic data at 525 eV, with the photopeak and shoulder features delineated. RPs have been generated from events that interact in the horizontal boundary region between two neighboring pixels (grades 346) for both the shoulder (bottom left) and photopeak.
Events beneath the two gates held high (+5 V) contribute to the shoulder, while events beneath the gate held low (−5 V) contribute to the peak. Clearly, the p⁺ implant is not dead, as we had previously assumed.

Figure 4-17  Top: Monochromatic 525 eV spectrum of standard grade (i.e. 02346) events, showing the selection criteria for main peak (“Photopeak”) and shoulder (“Shoulder”) events. Bottom: Combined RP maps for all horizontally split events, including the 3- and 4- pixel events (grade 6) that are near the corner of a pixel. The shoulder events (left) are localized to regions beneath the two gates with positive bias, while the the photopeak events (right) only occur beneath the gate with negative bias.
Figure 4-18 SEM photographs of the front (left) and back (right) of one hole from the 1.4 µm × 1.4 µm mesh. The concentric features on the back of the surface result from the fabrication process. The bar at the bottom of each photograph is 1 µm.

4.9 IMPROVEMENT TO THE MESH TECHNIQUE

4.9.1 REFINED EXPERIMENTAL METHOD

Armed with our improved understanding of the charge loss mechanism, we refined our experimental method. The first change involved the mesh itself. While our previous results clearly imaged the different regions of the pixel, increased spatial resolution would afford higher precision measurements. We obtained a new mesh consisting of a 10 µm thin nickel film which has large (tens of microns), rectangular holes. These holes are then filled in, via electro-forming. The final result is a mesh with square holes 1.4 µm on a side. Figure 4-18 shows the front (left) and back (right) surfaces around one of these holes. The spacing between holes was also increased to 48 µm, a factor of two larger than the previous mesh.\(^5\) This mesh has transmission properties similar to the earlier one due to their nearly identical atomic numbers. In the 0.277 – 0.704 keV energy range of the new measurements, the transmission is less than 1 × 10\(^{-11}\).

\(^5\)Due to certain measurements not discussed in thesis, a spacing twice that of the pixel dimension is desirable. See, e.g., Tsunemi et al. (1999).
The next improvement involved changing the way the mesh was held fixed with respect to the CCD. We discovered that we could place the mesh virtually on top of the detector. Due to the finite distance between the X-ray and CCD, the gap between the mesh and detector should be as small as possible to reduce the broadening the spot size due to beam divergence and diffraction. Figure 4-19 shows the arrangement of the new mesh and CCD, while the right panel shows raw data with the moiré effect and count-rate variation clearly visible. Compare to Figures 4-1 and 4-3 (left).

![Figure 4-19 Improvements to the mesh technique. Left: Schematic showing the orientation of the new mesh with respect to the CCD. Compare with Figure 4-1 Right: Raw data obtained from the experimental set-up shown to the left. The intensity variation seen in the moiré pattern is due to attenuation by the sub-pixel structure. There is marked improvement in resolution compared to the previous results using the mesh with large holes shown in Figure 4-3 (left).](image)

The last change was in the source of X-rays. Before, we primarily used a photon fluorescence source whose spectrum contained a relatively large amount of continuum. Now, we exclusively use the IFM as the source of X-ray. This electron impact source and grating monochromator provide a spectrally purer source of X-rays than the HEXS. Elimination of contaminating spectral background removes any uncertainty in the origin of events outside the main photopeak and allows us to make an RP from events taken from the entire span of the spectral redistribution function. Figure 4-20 illustrates the resolution gained when these three refinements are applied to mesh experiment.
Figure 4-20 Mesh data taken at 525 eV. Top: Data acquired using the mesh with 4 µm holes. Bottom: Data obtained after refining the technique and using a mesh with 1.4 µm holes. In each case, the representative pixel (RP) has been repeated in a $3 \times 3$ array to show the change in detection efficiency across the pixel boundaries.
Figure 4-21 $3 \times 3$ arrays of grade 0, grade 2, grades 34, and grade 6 Representative Pixels (RP). Each column has the same energy, and each row has the same grade. The data are presented in increasing order of total attenuation length ($\text{Si} \times \text{SiO}_2$): C Kα (left), Fe Lα (middle), and O Kα (right). Low counting statistics account for the poor resolution of the grade 34 & grade 6 C Kα data.
Using the new mesh, a series of measurements were made at energies of 277 eV, 525 eV and 704 eV, corresponding to the emission lines of C Kα, O Kα, and Fe Lα, respectively. Figure 4-21 displays RPs generated from various grades (02346) drawn from the entire SRF. (For additional comparison between the two implementations of the mesh technique, see Figure 4-4). Due to the low characteristic absorption lengths at 277 eV, the detection efficiency at C Kα is quite low, particularly over the channel stops. The relatively sparse data results in the course resolution of the horizontally split 2-pixel events (g34) and 3- and 4-pixel events (g6).

4.9.2 Data Analysis and Results

For the analysis below we only consider the measurements made at 525 eV and 704 eV, as a second CCD gate structure different from the first, was used for the measurement at 277 eV. The first step is to calculate the decrease in detection efficiency due to attenuation by channel stop. Unlike the previous experiment, RPs were generated using events drawn from the entire SRF. We use the same five-parameter channel stop model as before (Figure 4-6) and approach, i.e. generating an AF, folding the convolution of the model and AF through the data, and minimizing $\chi^2$. Figure 4-22 shows the attenuation due to the channel stops.

A convenient way to understand the best-fit data is to take slices through the multi-dimensional parameter space parallel to the plane of two related parameters, e.g. Si and SiO₂ thickness. Figure 4-23 shows contour plots for each energy. The 68% and 99% confidence limits are drawn and the best-fit value is denoted by the star. The degeneracy between the two parameters is easily understood as the model cannot differentiate between attenuation by purely Si or SiO₂ or some combination of both.

However, by simultaneously fitting the data at these two energies, one below and one above the O Kα absorption edge (534 eV) where the ratio of characteristic

---

6 The first device suffered a failure after the first two experiments.
Figure 4-22 The RPs generated from 1.4 µm mesh measurements at 525 eV and 704 eV have been summed in the direction parallel to the channel stops. The drop in detection efficiency results from attenuation by the constituent materials of the channel stop.

absorption lengths are markedly different, the degeneracy can be broken. Figure 4-24 shows the combined contour plot. Table 4-3 shows the range of parameter space searched and the best-fit values.

The 90% confidence limits encompass a tightly constrained region around the best-fit values of 0.0 µm (Si p⁺ depth) and 0.39 µm (SiO₂ depth). We note that, as expected we analyzing events taken from the entire SRF, the thickness of the p⁺ layer is zero. A similar analysis for the two width parameters yields best fit values of 4.3 µm for the box width and 0.3 µm for the wing width. We estimate systematic uncertainties to be ~10%.

While the measured value of 0.0 µm for the implant parameter is correct for data
Figure 4-23 $\chi^2$ contour plots for the Si p+ depth versus SiO$_2$ depth for data at 525 eV (left) and 704 eV (right). The contours correspond to the 68% and 99% confidence levels, and the star shows the best-fit value.

Table 4-3: Channel stops values derived from considering the entire SRF from under all the gates

<table>
<thead>
<tr>
<th>Name</th>
<th>Search range</th>
<th>Step size</th>
<th>Best-fit value</th>
</tr>
</thead>
<tbody>
<tr>
<td>box width</td>
<td>3.1 – 4.8 $\mu$m</td>
<td>0.16 $\mu$m</td>
<td>4.3 $\pm$ 0.3 $\mu$m</td>
</tr>
<tr>
<td>wing width</td>
<td>0.11 – 1.1 $\mu$m</td>
<td>0.12 $\mu$m</td>
<td>0.3 $\pm$ 0.1 $\mu$m</td>
</tr>
<tr>
<td>Si thickness</td>
<td>0.0 – 1.3 $\mu$m</td>
<td>0.08 $\mu$m</td>
<td>0.0$^{+0.04}_{-0.02}$ $\mu$m</td>
</tr>
<tr>
<td>SiO$_2$ thickness</td>
<td>0.0 – 1.3 $\mu$m</td>
<td>0.08 $\mu$m</td>
<td>0.39 $\pm$ 0.03 $\mu$m</td>
</tr>
<tr>
<td>Si$_3$N$_4$ thickness</td>
<td>0.0 – 0.05 $\mu$m</td>
<td>0.01 $\mu$m</td>
<td>insensitive</td>
</tr>
</tbody>
</table>

drawn from the entire SRF, we still have yet to determine the thickness of the Si p+ layer. This information can be obtained by carefully selecting only a portion of the RP data. As shown in Figure 4-17 (bottom), photo-absorptions in the channel stop implant under gates with high voltages contribute to the shoulder, not the photopeak. If we exclude that portion of the RP that contains the low gates (roughly one-third of the pixel) and only draw events from the photopeak of the SRF, the p+ layer is effectively dead. When we perform our fitting, then, we expect a non-zero value for the Si thickness. Again, we fit the two data sets simultaneously to break the degeneracy. Figure 4-25 shows the combined contour plot for Si and SiO$_2$ thickness. Table 4-4
Figure 4-24 $\chi^2$ contour plots showing Si p+ depth versus SiO$_2$ depth for the simultaneous fit of data taken at 525 eV and 704 eV. Data is drawn from the entire spectral redistribution function. The contours correspond to the 68% and 99% confidence levels, and the star shows the best-fit value.

lists the area of parameter space searched and the best-fit parameters derived from the photopeak data beneath the high gates.

The model now has best-fit values of 0.32 $\mu$m (Si p+ depth) and 0.47 $\mu$m (SiO$_2$ depth). Systematic uncertainties are now estimated to be $\sim$20%, a factor of two larger than before since only a subset of the data is being considered. The difference derived for the oxide thickness in the two analyses are entirely consistent with one another, given the measurement errors. Finally, we note that box width derived in this case is slightly narrower ($\sim$0.3 $\mu$m smaller) than the values determined when using the RP generated from the entire span of the SRF. This result is not entirely unexpected, as two-dimensional modeling of the potential fields beneath the channel stops indicates
Table 4-4: Channel stops values derived from considering only the photopeak events under the high gates.

<table>
<thead>
<tr>
<th>Name</th>
<th>Search range</th>
<th>Step size</th>
<th>Best-fit value</th>
</tr>
</thead>
<tbody>
<tr>
<td>box width</td>
<td>3.1 – 4.8 μm</td>
<td>0.16 μm</td>
<td>3.8^{+0.4}_{-1} μm</td>
</tr>
<tr>
<td>wing width</td>
<td>0.11 – 1.1 μm</td>
<td>0.12 μm</td>
<td>0.1 ± 0.1 μm</td>
</tr>
<tr>
<td>Si thickness</td>
<td>0.0 – 1.3 μm</td>
<td>0.08 μm</td>
<td>0.32^{+0.07}_{-0.03} μm</td>
</tr>
<tr>
<td>SiO₂ thickness</td>
<td>0.0 – 1.3 μm</td>
<td>0.08 μm</td>
<td>0.47^{+0.01}_{-0.08} μm</td>
</tr>
<tr>
<td>Si₃N₄ thickness</td>
<td>0.0 – 0.05 μm</td>
<td>0.01 μm</td>
<td>insensitive</td>
</tr>
</tbody>
</table>

that the strong lateral fields present at the edge of the implant region may sweep out charge before it has a chance to experience charge-loss at the p⁺ implant–SiO₂ interface. This would effectively reduce the width of the implant, as measured with our current analysis. In our future implementation of the mesh technique, our channel stop model will have independent variables for the width of the oxide layer and Si p⁺ region.
Figure 4-25 \( \chi^2 \) contour plots showing Si p+ depth versus SiO\(_2\) depth for the simultaneous fit of data taken at 525 eV and 704 eV. Only data from the photopeak has been used in the region of the pixel where the gate voltages were +5.0 V. This particular subset of data ensures that the doped p+ region will effectively be dead for this analysis. The contours correspond to the 68% and 99% confidence levels, and the star shows the best-fit value.