Sub-pixel event repositioning algorithms for Chandra X-ray astronomical imaging

Jingqiang Li

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Joel Kastner  
Joel H. Kastner, Ph.D., Dissertation Advisor

Harvey E. Rhody  
Harvey Rhody, Ph.D.

Zoran Ninkov  
Zoran Ninkov, Ph.D.

P. Bajorski  
Peter Bajorski, Ph.D.

May 4, 2004

Date
Title of Dissertation:
Sub-pixel Event Repositioning Algorithms for Chandra X-ray Astronomical Imaging

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Signature  Jingqiang Li  May 5, 2004  
Date
Chandra X-ray Observatory (CXO) with the Advanced CCD Imaging Spectrometer (ACIS) offers unprecedented spatial resolution for X-ray astronomical imaging. As focal plane arrays, ACIS CCDs were fabricated to satisfy CXO's requirements in spatial and spectral specifications, and operate in photon-counting mode to record any photoelectric interactions into event lists with energy information and charge split morphology (grade). The charge cloud generated by a single X-ray photon has a relatively small size compared to ACIS pixel, and the shape is approximated by an axial-symmetric Gaussian with full width half maximum (FWHM) about 2 to 4 microns. This fact indicates that the impact positions of photons that generate split events are near the pixel boundaries, instead of the pixel centers. Considering ACIS CCDs have pixel size of 24 microns, subpixel event repositioning (SER) algorithms designed to refine the positions of split events should significantly improve the spatial resolution of Chandra/ACIS imaging. SER methods have been modified, from original corner-split events only model, to static SER (including 2-pixel and single pixel events), energy-dependent SER, and charge-split dependent SER, for both backside-illuminated (BI) and frontside-illuminated (FI) CCDs. Both simulated and CXO-observation data demonstrate the improvement for various SER methods. Chandra/ACIS data obtained for the
Orion Nebula Cluster (ONC) was used to evaluate the SER algorithms, by reconstructing point-like sources in ONC and measuring their FWHM before and after applying SER methods. The improvement of FWHM for simulated and ONC sources was analyzed, so as to establish the degree of image improvement achieved by, as well as limitations on the success of, subpixel event repositioning algorithms. BI and FI CCDs exhibit different performance and, overall, BI applications benefit more from angular resolution improvement after applying SER techniques. The best performance after applying SER techniques can be as much as 62%, i.e., very close to theoretically available improvement, depending on applied SER method, source spectrum, off-axis angle, and employed CCD type.
Acknowledgements

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<td>ASCA</td>
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<tr>
<td>AXAF</td>
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<td>Backside Illuminated</td>
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<td>FI</td>
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<td>Flexible Image Transport System.</td>
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<td>Field of View</td>
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Chapter 1

Introduction: Basic Principles of X-ray Imaging

Astronomy, the scientific study of matter in outer space, started with exploring celestial objects and progressed after Galileo first used the telescope. Astronomers are dedicated to constructing larger telescopes in order to obtain greater collection power and better viewing conditions to study fainter and more distant targets. However, this effort until fairly recently was limited to visible light. Only when the invisible radiation from the stars was detected and measured after the middle of the 20th century, such as radio waves, infrared, and most recently ultraviolet, X-ray and gamma rays, the Universe disclosed a new vision to the world.

The fact that different spectral ranges allow different and complementary insights of the Universe promises X-ray astronomy to be a powerful approach of exploring cosmic events. X-ray astronomy covers a band of photon energies between 0.1 keV and 500 keV, and became the most fruitful among the newly opened spectral ranges during the last five decades\(^1\). X-ray astronomy makes observations in the higher-energetic radiation of the electromagnetic spectrum; studied objects include the sun and other normal stars, but also

\(^1\)http://wave.xray.mep.mpg.de/general/profile
extend to quasars at the edge of the Universe (Culhane & Sanford 1981).

1.1 X-ray Radiation

X-rays are a form of electromagnetic radiation similar to visible light, but have shorter wavelength thus higher energy. Because of their high energy, they cannot be handled by lenses and only reflected with very stringent conditions. However, because of their high energy, particular electronic detectors can register X-radiation by counting single photons. This is why detectors based on the photon counting approach are most commonly used in X-ray astronomy.

The sun is our nearest and most intense X-ray source. The detection of X-rays from the sun by a photographic plate detector covered by thin beryllium filters marked the beginning of X-ray astronomy in 1948 (Sanford et al. 1981). During the following more than 50 years, X-ray astronomy has developed into a “full fledged branch” (Bradt et al. 1992), in both theory and practical technique. Astronomers designed many satellites and missions dedicated to X-rays and were able to focus on many fascinating celestial objects.

X-ray emissions are produced by hot and violent processes, resulting from cosmic objects under extreme conditions. Therefore, X-ray sources are usually extremely variable, and are generally related to hot universe and nuclear energy process. The X-ray band includes the K-shell transitions (i.e., energy levels n=2 to 1) of all elements heavier than He. The X-ray continuum shape also provides important clues to high-energy emission processes.

1.2 X-ray Detection

"X-ray astronomy is the product of Space age."1

The opaqueness of the atmosphere prevents high energy electromagnetic radiation from reaching the Earth’s surface, and forced the development of the branches of astronomy based on high energy to wait for the availability of space vehicles that carry detection equipment
above the absorption layers. Balloons, sounding rockets and satellites are the transportation tools to lift scientific payloads up to different heights (Culhane & Sanford, 1981).

The balloon-borne instrument can detect incoming radiation only at energies above 20-25 keV, because balloons can only remain at heights of around 30 kilometers for a period of 48 hours. This energy range definitely enhanced the understanding of the world, but limited significant discoveries as well, because of lack of access to the important energy range of 1-10 keV (Culhane & Sanford 1981).

Various vertical sounding rockets have been used to study X-ray radiation from the Sun and other cosmic sources during the past fifty years. Compared with balloons, the rockets have both advantages and disadvantages. They can reach as high as 120 km to carry instruments for softer X-ray observations, but they can only remain at astronomically useful altitudes for a few minutes. Nevertheless, X-ray astronomy owes much progress to the observations made with rocket-borne instrumentation (Culhane & Sanford 1981).

Orbiting satellites can remain at their operational altitude up to few years. The satellites dedicated to X-ray astronomy have long stable continuous observation ability and provided vast quantities of archived data to the world, including all-sky X-ray imaging surveys.

1.3 X-ray Satellite Missions

The following will briefly introduce non-solar (intentionally or not) X-ray missions in the past four decades. One can see the great improvement of both the detector sensitivity and telescope resolving power.

The first satellite that detected cosmic X-ray radiations, the Third Orbiting Solar Observatory (OSO-3), was launched in 1967. Its imaging instrument had an energy range from 7.7 to 210 keV with six channels, with energy resolution of 45% at 30 keV

Uhuru was the first earth-orbiting mission dedicated entirely to celestial X-ray as-

\[^2\text{http://imagine.gsfc.nasa.gov/docs/science/how.l2/xray_detectors.html}\]
tronomy, and provided the first comprehensive view of the entire X-ray sky. The imaging instrument was two sets of proportional counters, which operated in the energy band of 2 to 20 keV.

The launch of the Einstein Observatory (HEAO-2) was a milestone for X-ray astronomy because its "scientific outcome completely changed the view of the X-ray sky". It was the first fully imaging X-ray telescope in space, with a sensitivity several hundred times greater than that of any previous missions. As a result, it was the first mission able to image extended sources (diffuse emission), as well as to detect faint sources.

Einstein had Wolter type I grazing incidence telescope that had a useful energy band from 0.2 to 4 keV, and four detector instruments that were sensitive to X-rays with energy range of 0.2 - 20 keV. The four imaging or spectral instruments could be rotated into the focal plane one at a time. Among them, the High Resolution Imager had the highest spatial resolution of ~2 arcsec, while the Focal Plane Crystal Spectrometer had the highest spectral resolution with E/ΔE of 50-100.

The Röntgen Satellite, ROSAT, was launched in 1990 and operated for almost 9 years. It had energy range of X-ray from 0.1 to 2.5 keV, and of XUV (Extreme Ultra Violet) from 62 to 206 eV. Using the Position Sensitive Proportional Counter detector, the first half year of the mission was dedicated from all-sky survey, and that was the first all-sky X-ray and XUV survey using an imaging telescope.

ASCA, the Advanced Satellite for Cosmology and Astrophysics, launched in 1993, was the first satellite to use CCD detectors for X-ray astronomy. ASCA has four X-ray telescopes with total effective area of 1,300 cm² at 1 keV. Its CCD arrays had field of view of 22' x 22', with spatial resolution of 30 arcsec, and energy resolution of 2% at 5.9 keV. These CCD detector arrays made ASCA the first X-ray mission to combine imaging capability and medium spectral resolution through a broad bandpass with a large effective area.

Chandra X-ray Observatory (CXO), renamed from Advanced X-ray Astrophysics Fa-
cility (AXAF) in honor of astrophysicist Subrahmanyan Chandrasekhar, was launched in July 1999. Chandra, as the successor to ROSAT, boasts the best (also the most expensive) X-ray telescope ever built. It is the first X-ray mission with the potential for sub-arcsecond spatial resolution.

Chandra has a single Wolter type I X-ray telescope with ghost-free field of view about 30 arcmin diameter and an effective area of 400 cm² at 5.0 keV. CCD arrays (ACIS: Advanced CCD Imaging Spectrometer) were employed as imaging instruments with ~ 0.5 arcsec spatial resolution, as well as dispersive spectrometers with spectral resolving power E/ΔE ~ 60-1000. Chandra/ACIS X-ray imaging offers the unprecedented spatial resolution and moderate spectral resolution simultaneously, and Chandra/HRC (High Resolution Camera) offers the best angular resolution of all the X-ray missions so far.

As a cornerstone of the European Space Agency’s science program, The X-ray Multi-Mirror satellite (XMM-Newton) was launched in December 1999. It is usually treated as the scientific-complementary facility of Chandra, with the energy range of 0.1 – 15 keV. Following the path of ASCA in providing greater mirror area but at lower resolution than CXO, XMM-Newton carries high throughput X-ray telescopes with an unprecedented effective area, and an optical monitor, the first flown on an X-ray observatory. The large collecting area and ability to make long uninterrupted exposures provide highly sensitive observations. Like ASCA and Chandra, CCDs were also employed in XMM-Newton.

1.4 X-ray Detectors

Parallel with the development of X-ray telescopes were the scientific equipments at focal planes designed to collect large numbers of X-rays from relatively bright sources to perform detailed spectroscopic and timing investigations.

The quest for X-ray astronomy is to detect a weak source against a relatively strong background. The relative weakness of a source makes integration detectors impractical as X-ray measurement instruments. So the detection is done upon a photon-by-photon basis.
Figure 1.1: The significant X-ray missions in the past forty years.
Therefore, X-ray detectors are counting individual photons in contrast to those in most other wavebands where accumulating incoming flux is common. As a consequence, the X-ray data usually comprise lists of events and their attributes, like arrival time, position, etc. Some detectors may offer spectral information as well as spatial information.

A wide variety of X-ray detectors have been developed, measuring the photon position, incidence time, and/or photon energy. The following sections briefly introduce different kinds of X-ray detectors commonly used in present and previous X-ray missions.

1.4.1 Proportional Counters

X-ray proportional counters (PCs) provide signals of the photon energies, interaction positions and arrival times. PCs consist of a windowed gas cell subdivided into different regions, and detect X-rays by photoionization of the counter gas. Position Sensitive Proportional Counter (PSPC) was uses on ROSAT.

1.4.2 Microchannel Plates

Used as efficient electron or low energy photon detectors, microchannel plate (MCP) detectors are compact electron multipliers with high gain. Even though a MCP has very high spatial and time resolution, it doesn’t have energy resolution, and has normally very low quantum efficiency. High Resolution Imager (HRI) on ROSAT and High Resolution Camera (HRC) on CXO are MCP detectors.

1.4.3 Semiconductor Detectors

Detectors based on silicon and germanium can have good energy resolving ability for single photons. Therefore, semiconductors, or solid state detectors, are used both for imaging devices and spectrometers, with desirable linear response, low noise, and moderate spectral resolution as well.

Charge coupled devices (CCDs) are now used in a variety of ways for X-ray imaging.
The latest missions, include ASCA, Chandra and XMM-Newton, have successfully explored the advantage of using CCDs as focal plane detectors.

1.4.4 Other Detectors

Phosphor X-ray detectors can be used for high resolution soft X-ray imaging by converting X-ray energy into visible light. Theoretically, phosphors can have the highest spatial resolution of all photon counting X-ray imagers – but have yet to be employed in any practical sense.

As one type of X-ray detectors, Scintillators (like Gas Imaging Spectrometer [GIS] on ASCA) are based on conversion essentially similar to these using phosphor, but are distinguished by the materials employed.

Negative electron affinity detectors (NEADs) were discussed as “a most promising new technology for X-ray detectors” in the late 1970s. NEADs were described as devices with highly desirable properties, with high spatial resolution, excellent quantum efficiency (near unity), and moderate energy resolution. However, one rarely even finds a reference to a NEAD in today’s literature.

Single photon calorimeters (SPCs) are actually very sensitive thermometers, and perhaps the most intriguing advance in X-ray astronomy instrumentation in contemporaneity. At the very low temperatures, the SPCs are able to get the best spectral resolution of any non-dispersive spectrometers.

1.5 X-ray Future

Is 50 years old still young for X-ray astronomy? No matter what the answer is, the truth is that during the past 50 years, X-ray astronomy has accomplished a billion times improvement in sensitivity, a quarter of a million times improvement in spatial resolution, and ten thousand times improvement in spectral resolution. Can this blossomy branch keep this progress up for the next five decades?
High resolution, high sensitivity spectroscopies like quantum calorimetry are very promising to significantly improve the energy resolving power. X-ray polarimetry and interferometry are popular topics too, since the former will offer a new way to look at the Universe and make surprising discoveries, while the latter will make micro-arcsecond imaging resolution possible.

In the mean time, the vast quantity of existing high-quality X-ray observations — especially those now being obtained by CXO and XMM-Newton— is the fortune of the whole astronomy community. Analysis on these archived data can provide an outline for future studies. New data analysis techniques that maximize the information content in these X-ray images will be required to fulfill this great potential.
Chapter 2

Overview of Chandra X-ray Observatory and ACIS

The Chandra X-ray Observatory, formerly the Advanced X-ray Astrophysics Facility, combines great spatial and spectral resolution, large image collecting area, and high sensitivity together into one package. After launch and deployment by the Space Shuttle Columbia on July 23, 1999, Chandra was boosted into an elliptical high-earth orbit to obtain the capability to study extremely faint sources by long-duration uninterrupted exposures.

The efficient high-resolution X-ray telescope and a set of advanced imaging and spectroscopic instruments make Chandra itself complex. Many subsystems, like pointing and dithering, data capturing and on-board processing, make it the most sophisticated X-ray observatory ever built.

The scientific instruments, including optics, detectors, gratings, and operation control, are the essential elements of the CXO. The following sections will briefly introduce those components; interested readers can find detailed information at the Chandra Proposer’s Observatory Guide 

\(^5\)http://cxc.harvard.edu/udocs/docs/POG/MPOG/
2.1 HRMA

Total reflection is a process that occurs when Snell’s law for refraction \((\sin[i]/\sin[r] = \mu)\), here \(\mu\) is refractive index) can no longer be solved for real angles. Visible light can achieve total reflection at the interface of two different mediums; so can X-ray beams. However, for a vacuum-metal interface, the refractive index is 0.9994, very close to unity. Therefore, the critical angle of grazing incidence has to be less than 2° to ensure total external reflection (Culhane & Sanford, 1981).

In addition to reflection, optical light rays can penetrate and refract through an optical lens to focus an image. Because of high energy, X-ray beams cannot do this, in other words, X-ray images cannot be formed by redirection by an optical lens. Therefore, X-ray focusing has to depend on reflection, and only at grazing incidence.

Based on this principle, the Wolter-I type image-forming system employs two reflections, first from a paraboloid and then a hyperboloid, to minimize the aberrations associated with a single reflection. Figure 2.2 illustrates the design schematically.

Chandra’s High Resolution Mirror Assembly (HRMA) (figure 2.3) consists of four pairs
of such Wolter-I type mirrors and their support structures. The iridium-coated mirrors are concentrically nested to focus photons with energy from 0.1 to 10 keV. The successful design, fabrication and alignment of Chandra’s nested mirror shells give the HRMA unprecedented angular resolution of one half arcsecond.

2.2 SIM

The Science Instrument Module (SIM) is a movable bench placed at the focal plane and housing the X-ray detectors, including both ACIS and HRC. SIM can move along the optical axis to adjust the telescope’s focal length, and orthogonal to it for imaging instrument and aimpoint selection. SIM’s movement can be as fine as 25 microns in the direction parallel to the telescope’s axis, and 250 microns perpendicular.
Because there are three fundamental coordinate systems in the CXO event list, i.e., Chip, Detector, and Sky coordinates, and each principle imaging component has a fixed orientation and position relative to the SIM, SIM's position and movement are recorded to provide critical information for the conversion between any two of the three coordinate systems.

### 2.3 ACIS

The Chandra Advanced CCD Imaging Spectrometer (ACIS) is one of the two imaging instruments at the HRMA focal plane. As the name suggests, it is made of Charge Coupled Devices, specially designed for X-ray imaging. ACIS consists of 10 single CCD chips, all identical in format (1024 × 1024). Two of them are backside illuminated (BI) while the other eight are frontside illuminated (FI). Each chip is a 3-phase, frame transferred CCD.
The 24 \( \mu \text{m} \) CCD pixel size is equivalent to \( \sim 0.5 \) arcsecond angular resolution. As shown in the ACIS layout (figure 2.4), each chip has two parts: the light color is the imaging section, while the dense color is frame store section. Four chips, I0 to I3, abut into a \( 2 \times 2 \) array (ACIS-I) to image extended sources. The other six form ACIS-S and are designed as the primary detector for the High Energy Transmission Grating (HETG). Among them, S1 and S3\(^6\) are backside illuminated CCDs, intended to improve quantum efficiency at low energy.

![ACIS layout diagram](image)

Figure 2.4: The layout of ACIS at Chandra focal plane. There are ten individual chips; each has an imaging part (white) and storage part (shaded). The black dots indicate the first pixel in each chip (from CPOG).

ACIS offers great spatial resolution (\( \sim 0''.5 \) per pixel), and simultaneously performs medium resolution spectroscopy \( (E/\Delta E = 10 \sim 60) \) over almost the entire Chandra bandpass, with high quantum efficiency. This spectroscopic imaging capability is one of main advantages of using CCDs as the X-ray imaging instrument.

\(^6\)S3 is frequently used for imaging due to its favorable orientation when placed at the telescope boresight.
2.4 HRC

High Resolution Camera (HRC) is the other imaging instrument at Chandra’s focal plane aside from ACIS. HRC uses Micro-channel plates (MCP) technology that was used by Einstein and ROSAT. Like ACIS, HRC has an imaging array (HRC-I) and a spectroscopic array (HRC-S). The former is a monolithic square MCP with the field of view (FOV) of $30' \times 30'$ with the pixel size of 0.13 arcsec in both directions, offering potentially the highest angular resolution among X-ray missions. The latter is a long array that consists of three smaller chips, and serves as a readout for the Low Energy Transmission Grating (LETG).

The HRC arrays are complementary to ACIS. They extend the response to energies below the sensitivity of ACIS, and offer the best time resolution (16 ms). However, because MCPs do not lend themselves well to further imaging improvement beyond that already obtained via standard data processing, HRC will not be considered further in this thesis.

2.5 HETG and LETG

HETGs and LETGs, respectively, stand for High Energy Transmission Gratings and Low Energy Transmission Gratings, and are the two instruments on board Chandra dedicated for spectroscopy. The spectrometer works when one assembly swings into the position behind the HRMA. These gratings on the assembly diffract the X-ray photons reflected from the mirrors, changing their directions by amounts proportional to the photons’ energies. On the focal plane, the detectors record the locations of the diffracted photons, providing the information to precisely determine their energies. Figure 2.5 shows the on-position grating and its readout by ACIS-S. Study of improvement of HETG/LETG spectral resolution is beyond scope of this thesis, but is an open area for future research.
Figure 2.5: The Grating on position and its readout schematics. (Figure from http://chandra.harvard.edu/about/science_instruments2.html)
Chapter 3

The Ingredients of Sub-pixel Event Repositioning for Chandra X-ray Imaging

Several factors make SER feasible for Chandra/ACIS imaging. They are briefly listed below. The detailed explanation will be discussed in the following sections.

1. Multiple charge from one photon. A major difference between an X-ray photon with an optical/infrared photon is the much higher energy, and therefore higher electrons yield upon interaction with CCDs.

2. Photon Counting mode. Because multiple charge can be collected from a single photon, and the charge signal is much higher than the readout noise level, counting individual photons can be an alternative to photon accumulating as a recording method.

3. Photon energy. Because of the linearity of the CCD response, a photon energy can be estimated simply from the CCD gain and readout signal in the photon counting mode. In ACIS, the uncertainty of the energy estimation $E/\Delta E$ is about 50. Later we show that photon energy is very useful to improve photon impact position certainty.
4. Charge cloud size and CCD pixel size. The charge cloud size is relatively small, compared to ACIS pixel. Therefore when a photon was absorbed near a pixel center, most likely the charge will be deposited within that pixel only. However, if a neighboring pixel received partial charge from a photon, we could claim that the photon lands very close to the split boundary.

5. Event Grade. An event is a photon detection. A 3x3 pixel island is typically used to collect event signal. The event grade is a number generated from a bit map of the pixel island, and describes the charge split information and morphology.

6. PHAS. PHAS is the pulse-height amplitude column in the event lists stored by Chandra data processing tool, normally a 3 x 3 array of bias-corrected pixel pulse heights for the event island. This 9 element vector contains the event island pixel values, providing the information of charge split proportion in each island pixel.

7. Chandra's intentional dither motion. During an observation period, Chandra intentionally moves its pointing direction, following a Lissajous pattern. The dithering is mainly to minimize the effect of gaps between CCD chips, but it accidentally forces the photons even from a point source to uniformly land at different pixels and subpixel positions. Therefore all kinds of event grades can be formed.

8. CCD under-sampling. ACIS CCDs under-sample the PSF of the telescope, whose FWHM (Full Width at Half Maximum) is comparable to the CCD pixel size. This means that Chandra's spatial resolution of on-axis imaging is limited by ACIS physical pixel size (24.0 µm ≃ 0.492 arcsec), not the telescope itself. The fact of under-sampling motivates the development of the subpixel event repositioning algorithms in this thesis, to minimize the pixelization effects.
3.1 ACIS Overview

Inherently a CCD is a sampled analog device, a light-sensitive semiconductor device collecting signals when photoelectric interaction takes place. On a “dopant contaminated” silicon substrate, the device forms its own functional sections like gates, channel stops, buried channels, etc. Different fabrication procedures like dopant, oxidization, etching and annealing make the silicon wafer grow. Applied external voltage forms depleted regions to collect charge, and clock timing helps to read the signal out serially.

ASCA was the first X-ray mission to utilize CCDs as focal plane detectors. The advantage of using CCDs comparing to traditional imaging methods was demonstrated during this mission. Beside the linearity, high quantum efficiency, and low noise, CCDs can offer X-ray detection with both spatial and spectral resolutions simultaneously.

ACIS CCD arrays share the technological heritage with ASCA focal plane arrays, but have smaller pixel size (27 to 24 μm), and bigger single chip size (ASCA: 512 by 512; ACIS: 1024 by 1024). ACIS CCDs, which were fabricated by MIT Lincoln Laboratory (CCID-17 devices), have been optimized for high detective efficiency (QE: 0.2-0.9), superior energy resolution (E/ΔE ~ 10 – 60), and excellent spatial resolution (24 μm represents ~ 0.5 arcsecond on the sky) (Burke et al. 1997). The CCD has two sub-sections; one is active to image incident radiation, the other is for storage only. This shielded frame-store architecture design allows fast charge transfer from image section to storage section. The latter is then slowly read out during the next integration cycle to maximize the readout time and minimize any negative readout effects. Figure 3.1 schematically shows the structure of an ACIS CCD. Note that the device is served by four amplifier nodes which are usually operated in parallel. This design allows the charge to be clocked in either direction, and makes possible non-standard read-out configurations.

However, as X-ray energies drop below about 1 keV, the absorption length becomes very short (see figure 3.5), and a significant amount of radiation will be absorbed by the
dead-layers — the polysilicon and insulator layers on the device surface. One feasible solution to improve the low quantum efficiency at soft energy band is backside illumination. ACIS has ten CCD detectors, two of which are back-illuminated, while the other eight are front-illuminated.

![Image Section](Image)

Figure 3.1: Schematic of an ACIS CCD. Both imaging and framestore sections have 1026 rows and 1024 columns.

3.2 ACIS CCD Pixel Physical Properties

ACIS CCDs are fabricated on high-purity p-type silicon wafers with resistivity of about 7000 $\Omega\cdot$cm (Weisskopf et al. 1995), which offers deep depletion depth that is essential for good spectroscopic performance at higher X-ray energies, and low recombination losses which are required for high detective efficiency.

The ACIS CCDs are three-phase CCDs, which means the pixel structure is physically
Figure 3.2: The schematic top view of an ACIS pixel. A pixel can be defined by 3 gates and 2 channel stops. The dashed lines indicate ideal pixel boundaries.

defined by an area between two adjacent channel stops and three neighboring gates. The boundaries are completely defined by the structure implanted and grown on top of the nearly pure, high resistivity silicon. In one (horizontal) direction (see figure 3.2), the vertically elongated channel stops help define a potential barrier that serves as the boundary between the pixels. It is safe to assume that the boundary lies in the middle of the channel stops. In the other (vertical) direction, the boundary definition is dependent on the applied gate voltage. The overlapping between the gates, as well as the slightly different width among the three gates, will complicate the exact location where the boundary and pixel center are. For example, in flight ACIS applies low voltage (+2 volts) on gate 1, and high voltage (+12 volts) on gate 2 and 3 (see figure 3.2). The vertical boundary in this case should approximately be the middle of gate 1, and pixel center lies at the center of the boundary between gates 2 and 3. If a different voltage scheme is employed, the boundary location will change and will lie underneath a different gate. Therefore the following definitions were adopted (in Chip Coordinates):

- **vertical boundary:** the boundary formed by gates. In this thesis, the gates in ACIS chips are assumed to lie in horizontal configuration, as shown in figure 3.2.
Figure 3.3: The generic structure of ACIS BI and FI CCD devices. Photons come from the top in this diagram; slabs are not to scale. Label “ff” stands for “field free”. The diagram is from Townsley et al. (2002a).

- horizontal boundary: the boundary formed by channel stops. It was assumed that channel stops run vertically, perpendicular to the gates, as shown in figure 3.2.

Top view of the CCD surface (figure 3.2) gives pixel boundary and pixel structure. The physical difference between pixel gates and channel stops results in the non-uniformity within a pixel.

A cross-section of the CCD would show that there are many layers within a pixel. Townsley et al. (2002a) simplify ACIS FI CCDs into three layers, i.e., gates, depletion region, and bulk substrate, while BI CCDs have damage layer, epitaxial field free layer, depletion layer and gates, according to the incident photon direction. Figure 3.3 schematically illustrate both FI and BI ACIS CCD structure.

On the top section of the FI device is the gate layer, often referred to as dead layer. The gate section includes polysilicon and insulators as shown in figure 3.3 and 3.4. Photons that interact in this layer can produce secondary fluorescent photons that can be absorbed in depletion region and contribute substantially to the Si Kα peak (Townsley et al. 2002a).
Depletion region, often called active layer, is under the gates but interrupted with channel stops and buried channel. Channel stops serve as pixel boundaries, as mentioned before, while the buried channel is for holding charge signals and clocking them out efficiently. They only account for a small amount of depletion region. Photon interaction in the depleted slab is most desirable, since the nearly-uniform electric field in this layer sweeps the efficiently-generated electron charge cloud towards the gate.

In a BI device, the top layer is the “damage” slab defined by Towsley et al. (2002a), which is actually the back surface (often SiO2) to strengthen the thin CCD, left after the bulk substrate has been etched away. The following epitaxial field free region acts as a reflecting layer, and keeps the charge cloud generated in the active layer from leaking into the back surface. However, these two slabs are very thin compared to the depletion region; the latter makes up most of the thickness of the device, and functions as a high efficiency active area. The structure and function of both depletion zone and the gates layer in BI devices are the same as the FI devices, except that the thickness of depletion region is smaller.

### 3.3 Photoelectric Interaction

As an X-ray detector, a CCD records the signature of an X-ray interaction, and extracts the signal amplitude at the end of an exposure interval. The photon propagation, interaction and charge collection processes are dependent on photon energy, CCD structure and operating conditions, as well as where the interaction takes place. Without loss of generality, in the following analysis, it was assumed that an ACIS FI CCD, under default in-flight operating conditions, is illuminated by X-ray beams.

#### 3.3.1 Photon Propagation

The default applied voltage indicates that when ACIS CCDs were used to detect X-ray sources, gate 1 was held low, and gates 2 & 3 were held high during exposure time. If a
photon interacts under gates 2 or 3, the charge will more likely stay in just that pixel. If it interacts under gate 1, where the applied voltage is lower than other two gates, the charge will move to lower potential well\(^7\). This charge is easily split between at least two pixels. Likewise, if a photon interacts further into the silicon directly in the center of the pixel, charge can still be split into two neighboring pixels because of diffusion. This is where event grades are derived (see section 3.4).

ACIS FI chips have much more silicon than BI chips; i.e., FI devices have several hundred microns of bulk silicon beneath the gates. As the gate voltages go higher, one can deplete more of the device. Thus, for +2 (gate 1) and +12 (gates 2 & 3) volts, the depletion depth is around 70 microns. The higher the depletion depth, the bigger the quantum efficiency (QE), which relates to the photon attenuation length\(^8\).

\(^7\)Because the majority charge is electron for ACIS devices, higher voltage means lower potential.

\(^8\)Note: Attenuation length and absorption length are interchangeable in the literature.
The propagation length of photons in a single uniform slab can be characterized by transmission and absorption. An energy-dependent linear absorption coefficient of the material, \( \alpha \), parameterizes the transmittance \( T \) of the slab by:

\[
T(E) = e^{-\alpha(E)d}
\]

(3.1)

where \( E \) is the photon energy and \( d \) is the thickness of the material.

The attenuation length \( \lambda \) of a material is defined as the distance when half of the photons were absorbed. Therefore,

\[
\lambda(E) = -\frac{1}{\alpha(E)} \ln(0.5)
\]

(3.2)

The simple model for quantum efficiency is that any photon that interacts within the depletion depth will get detected (M.J. Pivovaroff: private communication). By assuming the depth of depletion zone as \( d_d \), the fraction of absorbed photon will equal to \( QE \):

\[
QE = 1 - e^{-d_d/\lambda(E)}.
\]

(3.3)

ACIS FI CCDs can have depletion depths as long as 70 µm (Prigozhin et al. 1998a) when applying default +2 and +12 volts voltage. At high energy, where a photon’s attenuation length is bigger than or comparable to the depletion depth \( d_d \), QE is very low since few photons will be absorbed inside the depleted region. As photon energy goes lower, with the absorption length smaller than \( d_d \), QE is close to unity since most photons will interact in the depleted zone. As photon energy goes even lower, the attenuation length is even smaller, and one might think that the QE tends toward unity. However, as the attenuation length gets smaller as the energy decreases, there’s now a non-zero chance that the photons can get absorbed in the gates or channel stops. The photons getting stopped in these “dead layers” can not be detected\(^9\). That’s why FI CCD has lower quantum efficiency at lower energy. At higher energies, the gates are sufficiently thin that very few, if any, photons are stopped by them.

\(^9\)The channel stop P+ region effectively is field-free region, therefore the charge loss is due to charge diffusion and recombination.
Charge collection is the process of charge cloud movement after it was generated until it reaches the buried channel during the exposure time. The process includes charge cloud generation, i.e., the photoelectric interaction, and charge diffusion including drift. The most common formula that was used to calculate the collected charge cloud radius $r$ (see table 3.2 for definition) is:

$$r = \sqrt{r_i^2 + r_d^2}$$

where $r_i$ is initial cloud radius, $r_d$ is cloud radius due to the diffusion process. The collected charge cloud size closely relates to charge split morphology, thus to the spatial resolution.

The mechanism of charge collecting is very complicated due to the non-uniformity within a pixel. Different photon impact positions cause various charge collection consequences. From top view, photons can land close to the pixel center, or near the boundaries.
From cross-section view, photons can be absorbed within the gates, channel stops, depletion zone, or field free substrate.

The Initial Charge Cloud

A photon with energy of 1.1 to 3.1 eV (11,263 Å–4,000 Å), if absorbed by silicon, will generate a single electron-hole (e-h) pair. This spectral range covers the near infrared (NIR) and visible spectrum (4000-7000 Å). Energy greater than 3.1 eV will produce multiple e-h pairs when the energetic conduction band electron collides with other valence electrons. The average number of electrons generated for an incident photon with energy $E(eV) > 10 \text{ eV}$ follows

$$\eta_i = \frac{E(eV)}{E_{e-h}}$$

where $\eta_i$ is the ideal quantum yield (electrons per interacting photon) and $E_{e-h}$ is the minimum energy required to liberate an electron-hole pair, which for silicon is $3.65eV/e^-$ at room temperature (Janesick 2001, pages 26-27).

ACIS CCDs are operated at the temperature of $-120^\circ \text{C}$, at which $E_{e-h} = 3.71 \text{ eV} e^{-1}$ (Townsley et al. 2002a). $\eta_i$ is proportional to readout signal amplitude and the latter is used to measure the photon energy at photon counting mode. Soft X-ray photons have much higher energy than visible light photons. Upon absorption by silicon, this additional energy generates multiple e-h pairs in the CCD. The initial charge cloud is assumed to have a three-dimensional Gaussian distribution, with energy-dependent radius (in unit of $\mu m$) defined as (Pavlov et al. 1999; Townsley et al. 2002a):

$$r_i \approx 0.0062E_i^{1.75}$$

where $E_i$ is incident photon’s energy in units of keV, and $r_i$ is initial charge cloud radius in microns. This means the initial charge cloud is very compact, for example, a 5.9 keV photon can generate 1590 $e^-$ contained within a diameter of only 0.28 $\mu m$ (FWHM).

After the initial charge cloud was generated by photoelectric interaction, the cloud
itself has to migrate to the buried channel in order to be collected. This process is called charge diffusion.

**Charge Diffusion in the Depletion Region**

Let's first consider charge cloud propagation in the so-called depletion region, a zone depleted of free carriers by a voltage applied to CCD gates. There is a strong electric field that drifts the photoelectrons toward the buried channel, with high drift velocity. The drift time from where the charge cloud was generated to the buried channel can be approximated by:

\[ t = \frac{\epsilon}{\mu e N_A} \ln \left( \frac{d_f}{d_f - z} \right) \]  

(3.7)

where \( \mu \) is the electron mobility, \( N_A \) is the acceptor concentration, \( e \) is the electronic charge in unit of Coulombs, \( \epsilon \) is the permittivity of silicon \((1.044 \cdot 10^{-12} F/cm)\), \( d_f \) is the thickness of the field region, and \( z \) is the distance below the buried channel at which the charges were generated (Janesick 2001).

The charge cloud will expand radially during the drift time by diffusion. By assuming that the drift time is much less than the time it would take in field-free diffusion, the 1\( \sigma \) radius is \( \sqrt{2Dt} \), so the 2\( \sigma \) cloud diameter \( c_f \) upon collection is

\[ c_f = (32Dt)^{1/2} = \left[ \frac{32D\epsilon}{\mu e N_A} \ln \left( \frac{d_f}{d_f - z} \right) \right]^{1/2} \]  

(3.8)

\[ \mu = A_f T^{-\gamma} \quad \text{cm}^2\text{V}^{-1}\text{s}^{-1} \]  

(3.9)

where \( D \) is diffusion constant, \( A_f = 1.43 \times 10^9 \), \( \gamma = 2.42 \) (Townsley et al. 2002a). Examples of values and units of these constants are (Hopkinson 1987): \( D = 35\text{cm}^2\cdot\text{s}^{-1} \), with \( \mu = 1500\text{cm}^2\cdot\text{V}^{-1}\cdot\text{s}^{-1} \), \( N_A = 10^{13}\text{cm}^{-3} \) and \( d_f \sim 30\mu m \). At these certain conditions, \( c_f \) is 5.81 \( \mu m \) when \( z \) is 15 \( \mu m \). Note that equation 3.8 will not hold within a distance \( \sim (D\epsilon/\mu e N_A)^{1/2} \) of the depletion layer boundary because in that region the drift velocity is comparable to the velocity of thermal diffusion.
Diffusion in the Field Free Region

The bulk substrate below the depletion region is the field-free zone, in which the charge diffusion and recombination become more important when a photon interacts. It is more likely that only a fraction of the initial charge will reach the buried channel and be collected in this case.

Charge diffusion in this region is very complicated, and was explored in Janesick (2001), Pavlov et al. (1999), and Hopkinson (1987). However, the outcomes are slightly different according to different CCDs described in those documents. Interested readers can refer to those references for further detail.

3.3.3 Photon Impact Positions in Top View

When a photon interacts within a pixel and close enough to the pixel center, a charge cloud is generated and its size depends on the photon energy and where the photon was absorbed. If the interaction happens inside the depletion region, the charge cloud will drift to the device surface quickly due to the electric field applied on the gates. The charge will most likely stay within one pixel and form a single pixel event. If the interaction happens underneath the depletion region, the charge cloud will expand radially. Some change will move to the gate and finally be collected; some will move to bottom, and will recombine and get lost. Laterally diffused charge will recombine or be collected eventually, depending on surrounding forces and the diffusion time. However, single pixel event will most likely be formed, either because most charges are collected within the pixel, or the split amount is too small to exceed the split event threshold applied during (event detection) data processing.

When a photon interacts beneath a vertical boundary—the gate with lower state—the charge cloud will be collected without recombining. However, since the applied voltage under the boundary is relatively low, the charge will flow to adjacent gates with higher voltage (therefore lower potential). A split event is easily formed, although a single pixel event could be recorded too.
When a photon interacts beneath a horizontal boundary—the p\(^+\) doped channel stop region—the charge will drift to where there is a lower potential, and is easy to split into adjacent pixels and form a split event. Charge suffers severe loss here because the heavily doped p\(^+\) region is effectively field-free.

The region inside the p\(^+\) doped channel stop is effectively field free. Photoelectric absorption there will create an electron cloud which will spread out in all directions due to diffusion. Some will reach the surface and be accumulated, some will go to the wrong way and be recombined eventually.

The micro structure of a pixel is much more complicated than that described above. The three gates of a pixel have different sizes and overlap each other. The sizes of channel stops can only be approximately determined by experiments, and the shape of potential well can only be roughly estimated by Poisson analysis. Also, the amount of charge loss in p\(^+\) implanted channel stops is unexplored yet. Such investigation is only based on experimental analysis and statistical fitting. Because the CCD device itself is not uniform, the results don’t agree well between different experiments, and depend highly on the device’s working conditions.

3.4 Event Grades

Events are defined as any occasion in which there is a signal remaining in a CCD pixel above a given event recognition threshold after bias subtraction. Thus an event may be produced by X-ray photons, incident charged particles (cosmic rays), noisy electronics, stray optical light or defective CCD pixels, just to name a few sources. It is part of the scientist’s analysis task to determine how to maximize the utility of the data by appropriately selecting events so as to maximize the signal and minimize the background.

The charge diffusion and charge loss processes just described in previous sections also affect the effective detection efficiency of the CCD. This coupling operates mainly by way of
the "event-shape-based" event selection criteria which, as discussed above, are used to reject events for which charge collection is so poor that the event amplitude is a poor measure of the incident photon energy. If each and every event rejected on grounds of shape resulted from interactions outside the depletion region, then the effect of the selection criteria could be modelled into a straightforward "geometrical" way. In fact, the selection criteria are not perfectly efficient; they accept a fraction of events occurring outside the depletion region, and reject a fraction of events occurring in the depletion region.

As described in 3.3, a single X-ray photon can generate multiple e-h pairs and thus a large CCD signal. Consequently, detecting X-ray photons is not limited to integration modes of operation. Instead, a photon counting mode offers photon energy measurement, in addition to spatial information.

ACIS uses photon counting mode to record incident photons individually. This means in a 3 × 3 or even bigger isolated sub-array island, ACIS implicitly assumes that at most one photon was collected in one exposure frame. An event with assigned grade is registered when signals in the CCD are read out. The on-board analysis software examines every pixel in the full CCD frame and extracts each 3 × 3 event region (the isolated sub-array island) with bias-subtracted pixel values in which the center pixel value is a local maximum and also exceeds a given event threshold. The neighboring pixels are then compared to the bias-subtracted split-event threshold, either in-flight or via ground processing software, and the event grade is assigned. Default event threshold is 38 and 20 ADU (AD unit) for FI and BI devices, respectively, and the split event threshold is 13 ADU for both types.

The event grade is a code that identifies how many and which surrounding pixels are above the split threshold, i.e., the split pixel distribution (morphology). If surrounding pixels are all below the split threshold, the event was considered a single-pixel event; otherwise it is a split event, and the signals in adjacent pixels above split event threshold are added to the signal in the central (maximum) pixel, to calculate detected photon energy. So event grading only depends on the signal distribution morphology after photoelectric absorption.
Table 3.1: ACIS and ASCA grades. Note that the grade mentioned in this literature means ACIS grade, except explicitly point to ASCA. In addition, the author doesn’t intend to distinguish ACIS grade, flight grade or FLTGRADE.

However, the signal distribution results from where the charges were collected, and thus from where the photon interacted and how the charge cloud traveled.

Split-pixel events are registered by assigning a unique grade which depends on charge split pattern. The grade is recorded along with the event signal into the telemetry to indicate the splitting information.

There are two kinds of grading schemes employed by Chandra, ASCA grade and ACIS flight grade. The former has 8 grades (5 “good” and 3 “bad”) and is from the nomenclature of the ASCA CCD (SIS: Solid-state Imaging Spectrometer) instrument. ACIS FLTGRADE has 256 different values, and each one is a bit map of the split pixel distribution, as shown in figure 3.6. However, not every ACIS grade likely corresponds to X-ray events. In particular, we assume that soft X-ray photons will only deposit charges in less than four pixels, and exclude diagonal split events; most other grades likely are formed either by incident noisy particles or photon pileup. Therefore, only 13 ACIS grades are “viable” (table 3.1). Understanding ACIS flight grade assignments can be easier by referring to figure 3.6, and the relationship of the two grading schemes is given in table 3.1.

10 Actually recording the grade or not depends on telemetry mode:
“faint” : 3 x 3 event island telemetered (no on-board grade).
“graded” : just central pixel plus (on-board assigned) grade.
Figure 3.6: Schematic for determining the grade of an event from a $3 \times 3$ event island. The center pixel is event pixel, while any neighboring pixels that exceed split threshold are called split pixels. The event flight grade is assigned as a bit map of the island.

3.4.1 Chandra’s Dither Motion

In contrast to typical satellite observatories, which point to a single direction during integration time, Chandra intentionally but slowly moves its pointing direction during an observation. This dither motion of the observatory moves the target across the CCD surface, in principle forcing the photons from a point source to

1. avoid impacting on single pixel, therefore minimize CCD non-uniformity and chip gap effects;

2. randomly land at different subpixel positions within the CCD pixels, therefore form all types of event grades.

The dither movement has a form of Lissajous figure, with a specific amplitude and period, and causes a non-extensive source to produce all kinds of event grades. This offers the opportunity of subpixel event repositioning algorithms, which depend on the split events, to be successfully applied on any X-ray sources.
3.5 Charge Cloud: Properties Deduced from Mesh Experiments

Both single- and multi-pitch mesh experiments (Tsunemi et al. 1999a) were used to analyze the charge cloud shape and size. A parallel X-ray beam with specific energies, CCD camera and metal mesh were used in the experiments. The metal mesh has relatively small holes periodically spaced a few CCD pixel widths apart, and was placed just above the CCD surface, parallel but with a small tilt angle. The tilt angle enables moire pattern, determines the alignment, and forces mesh hole and CCD pixel changing relative positions (Pavlov et al. 1999, Tsunemi et al. 1999a).

The experiment enables one to determine the photon impact position limited by mesh hole size. Because of moire pattern, mesh holes have slight different position relative to CCD pixels. From event grade, it is possible to estimate the final-charge-cloud (FCC) size, with the effect of mesh hole size. The charge cloud here is the convolution of mesh hole with collected-charge-cloud (CCC), i.e., the expansion (diffusion) of initial-charge-cloud (ICC). See table 3.2 for charge-cloud related definitions.

The deconvolution of the final-charge-cloud with the mesh hole is the collected-charge-cloud after travelling to the device surface via the depletion region. CCC size is the goal for the experiments.

Experiments show that the collected charge cloud shape can be well estimated by axisymmetric Gaussian function. For the CCD used in experiment in Tsunemi et al. (2000), horizontal (parallel to gates) sigma is about 1.4 microns, while the vertical (parallel to channel stops) sigma is about 0.7 microns for 1.5 keV X-ray photons. FWHM is 3.29 microns and 1.64 microns, for horizontal and vertical directions, respectively.

Other experiments (Hiraga et al. 1998, Tsunemi et al. 1999b) using different CCD devices show the prominent charge elongation in the same direction too. Why are horizontal and vertical charge cloud sizes different? Tsunemi et al. (1999b) conclude that the electric
field inside the depletion region is not uniform, which comes from the non-uniformity within a pixel. Pixel boundary was defined by the clocking gates and channel stops, which have different electro-magnetic properties. The asymmetry of the electric field inside a CCD pixel leads to the drift process asymmetry. The nonuniformity of the electric field forces the final charge cloud to be axial symmetry. The asymmetry depends not only on the CCD itself but also on the operating conditions.

From the experiments, Tsunemi et al. (2000) found that the charge cloud size is almost independent of the charge travel distance in the depletion region. This means charge drift velocity is much larger than the diffusion speed in the depleted area, and the collected charge size almost only depends on the cloud size expanded in electric field free area. In other words, the size is highly dependent on where the photon was absorbed. However,
Table 3.2: Different charge cloud definitions

<table>
<thead>
<tr>
<th>Acronyms</th>
<th>Full Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ICC</td>
<td>Initial Charge Cloud</td>
<td>The charge cloud size immediately after photon interaction and before the charge diffusion.</td>
</tr>
<tr>
<td>CCC</td>
<td>Collected Charge Cloud</td>
<td>The charge cloud size when charge reaches buried channel and before readout process. CCC depends on initial charge cloud and charge diffusion.</td>
</tr>
<tr>
<td>FCC</td>
<td>Final Charge Cloud</td>
<td>In the mesh experiment, the measured charge cloud size. FCC is the convolution of CCC with the mesh hole size.</td>
</tr>
</tbody>
</table>

this is only true when depletion depth is small, and the conclusion will not hold for large depleted region, like ACIS CCDs at default operating conditions.

The experimentally-measured charge cloud size is comparable to or slightly bigger than the employed mesh hole size. Therefore, one can expect that no corner split events will occur from photons absorbed near the pixel centers, and no single pixel events occur near the pixel boundary regions.

A similar mesh experiment has been done using ACIS FI CCD (Pivovaroff et al. 1998). Pivovaroff et al. (1998) briefly described the experiment and conclusively proved that different grades come from different parts of the pixel where photon impacted. The results show that ACIS yields a large fraction of grade 0 (single pixel) events at low energies, especially for FI devices, but these events also have the most uncertainty at where photon impacted within a pixel. Corner split events are those that occur when photons land near the pixel corners. These are three or four-pixel split events, for which there is the most location certainty. However, FI ACIS devices do not yield many of these, and the energy accuracy is lower than for grade 0 events. However, because of the different physical property of BI CCDs, corner split events have much higher proportion in these devices. Therefore, observations with BI devices (especially S3) offer a better chance to improve the angular resolution.
The relative ratio of different grades is called branching ratios (described in detail in section 8.1). The branching ratio of multiple-pixel events increases as energy increases for front illuminated CCDs. This relates to the initial size of the charge cloud, as well as the penetration depth of the photon.

Figure 3.8, from ACIS calibration report\textsuperscript{11}, shows the Chandra HRMA encircled energy surfaces projected onto a schematic of subpixel locations. Both grids show a geometric area (computed from the branching ratios) for the different event grades at two different energies. The figure illustrates that at higher energies a smaller percentage of the pixel area can produce a grade 0. 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.

\textsuperscript{11}http://www.astro.psu.edu/xray/docs/cal_report/cal_report.html
Figure 3.8: HRMA encircled energy surfaces projected onto a schematic of sub-pixel locations. Figure is from ACIS calibration report\textsuperscript{11} (Figure 4.56).
Chapter 4

The Necessity for Sub-pixel Event Repositioning

The ACIS physical properties and Chandra operation modes provide the possibility for SER techniques. Is SER really needed in application to Chandra/ACIS imaging data? What ideally can the improvement be if one applies this technique? This chapter will address such questions from an image degradation perspective.

4.1 PSF

Point spread function (PSF) is a pulse response of an imaging system, describing the shape of the final image output produced by a 2-dimensional delta function (point source). The main effect of PSF is blurring the object detail, like a low pass filter, suppressing the high spatial frequencies. The PSF of an imaging system is the result of cascaded modulation by every independent component.

Chandra produces sharper images than any other X-ray telescope to date and therefore provides an opportunity for high-angular resolution studies of X-ray sources. The blurring of the Chandra PSF can be decoupled into three contamination sources: the mirror (HRMA) PSF, which is dominated by optical aberrations; aspect blurring, caused by errors of tele-
scope intentional dither motion and pointing reconstruction; and pixelization effects, caused by the finite size of detector pixels. The three parts are statistically independent. Reducing the PSF effect from any sources will decrease the PSF of the whole system, therefore in principle increasing CXO resolving power.

Mirror PSF and aspect blurring can be referred as telescope PSF, which is fixed and determined by HRMA aperture, aberrations, and telescope pointing and tracking accuracy. Therefore, there is no space to improve system PSF from the telescope (absent improved pointing information).

There is nothing one can do for the detector physical pixel size either. Fortunately it is possible to reduce the pixel size effectively by appropriate approaches, however, such as SER methods addressed in following chapters. These methods reduce the blurring due to pixelization effects, therefore reducing PSF broadening of the whole imaging system.

However, accurately evaluating the contribution to the PSF for each part is very difficult, because no one really knows the HRMA PSF size and aspect blurring factor, other than empirical results from ground and on-orbit calibration data. Fortunately, the purpose of this analysis is to quantitatively evaluate the potential SER impact of, and the measurement error in each stage can be neglected.

### 4.2 HRMA PSF Estimation

The best available model for HRMA response function so far is ChaRT (Chandra Ray Tracer), the SAOsac ray trace code, which was developed at CXC (Chandra X-ray Center) for calibration purposes. The model traces rays through the Chandra x-ray optics to produce a point spread function, for a point source at any off-axis angle with any energy or spectrum.

Simulating the HRMA PSF using ChaRT is the first step in obtaining a good estimation.

\[ \theta \]

The off-axis angle, \( \theta \), of a source is typically defined as the angular distance of its detector coordinates relative to detector center.

of the Chandra PSF for a given observation. The shape and size of the HRMA PSFs vary significantly with source location in the telescope field of view (FOV), as well as with the spectral distribution of the source. Because of the Wolter-I type design, the image quality is best in a small area centered at the optical axis. In fact, the mirrors were designed to produce images with better than one arc-second resolution; in particular to concentrate better than 85% of the energy at 0.277 keV within a one arcsec diameter (CPOG).

ChaRT simulations were carried out for on-axis soft X-ray sources with a monochromatic energy of 1.74 keV. However, the simulation only provides the photon spatial position, along with the photon trajectory. A further “detection” process has to be involved in order to evaluate the PSF at focal plane. Therefore, MARX (Model of AXAF Response to X-rays) simulation with an ideal detector is necessary (by setting the MARX internal dither blur factor to zero), to intercept ray beams at telescope focal plane. ACIS-S detector, with unit quantum efficiency, was used in MARX simulation, at its default position\textsuperscript{14}. Simulated results show that the mirror PSF is about 0.29 arcsec in FWHM, at default ACIS-S position, for the specified on-axis monochromatic (1.74 keV) source. The scatter plot of “detected” photons is shown in the most left panel of figure 4.1.

Note that the SAOsac model currently does not model the dither motion of the telescope, i.e., the blur due to satellite dithering is not included in ChaRT; and does not include residual blur from aspect reconstruction errors. This blurring is also an important factor in SER analysis, and will be addressed in next section.

4.3 The Aspect Blurring

The best guess for aspect blurring factor is 0\textquoteright\textquoteright.07 arcsec (in RMS — root mean square uncertainty). This estimation is from an analysis of 276 observations\textsuperscript{15}. Considering this value as standard deviation (sigma), the equivalent FWHM in Gaussian function is 0\textquoteright\textquoteright.165

\textsuperscript{14}Simulations show that, ACIS-S and ACIS-I arrays have different default focal position, therefore HRMA will have different PSF size at two focal planes. However, the size difference is very small.

\textsuperscript{15}See \url{http://asc.harvard.edu/cal/ASPECT/img_recon/report.html}
Convoluting HRMA and aspect blurring results in the telescope PSF.

The MARX simulation, by projecting the detected photon back to sky, gives the individual photon origin in Sky coordinates \([X, Y]\). Therefore, by knowing the aspect blurring rms factor, one can evaluate telescope PSF (the convolution of HRMA PSF and aspect blurring) via a random process (B.K. Ishibashi: private communication), instead of direct convolution, which typically involves FFT (Fast Fourier Transform) and may lead to unexpected errors. This process adds the blur uncertainty for each photon, by the equation

\[
\begin{align*}
X &= X' + Rn(s) \cdot A_{bf} \\
Y &= Y' + Rn(s) \cdot A_{bf}
\end{align*}
\]

where \(Rn\) is a pseudo-random number generator for a normal distribution, \(s\) is its seed value, and \(A_{bf}\) is aspect blur factor of the dither motion; \(X'\) and \(Y'\) are photon origin in Sky coordinates without aspect blurring, and \(X, Y\) are after blurring. Although the value of aspect blur is not always certain, 0''.07 is quite reasonable. The telescope PSF can be constructed from \(X\) and \(Y\) values, and the result (FWHM) shows 0''.427 for above simulated on-axis X-ray source with an energy of 1.74 keV. Scatter plot of telescope PSF was shown in the middle panel of figure 4.1.

### 4.4 Pixelization Effect

ACIS has square pixel of 24 \(\mu m\), equivalent to 0''.492 in angular resolution. The presence of pixel quantization and pixel randomization\(^ {16}\) have the effective “net Gaussian” blur of (adding in quadrature):

\[
B = \sqrt{(\sqrt{2} \cdot f \cdot P_{x})^2 + (\sqrt{2} \cdot f \cdot R_{m})^2}
\]

\(^{16}\)The CXC standard data processing randomizes the positions of events detected within a given pixel. This randomization is done to remove the instrumental “gridded” appearance of the data and to avoid any possible aliasing affects associated with this spatial grid. The default randomization is adequate for most users. See http://cxc.harvard.edu/ciao/threads/index.html for details.
where $B$ is the blur due to pixelization (the first term) and randomization (the second term) in the Sky X direction, $f$ is a converting factor and equals 0.29, $P_x$ and $R_m$ are pixelization and randomization terms, respectively, and both equal to 0.492 arcsecond. Therefore $B$ equals to $0''.285$. Both terms represent the blurring in unit of root-mean-square (RMS) radius (hence the pixel value is converted to its RMS radius equivalent by multiplying $\sqrt{2} \cdot f$ term). In the case where pixel randomization is turned off, the second term is set to zero. In SER application, the randomization was removed first. Therefore, the equivalent Gaussian blur factor of pixelization is $B = \sqrt{2} \cdot f \cdot P_x$.

Note that the term $f$ equals to 0.29, and is a “fudge” factor to convert the full 1-D width of a uniform distribution (e.g., pixel quantization) into the RMS radius equivalent of the distribution. Basically the RMS of a (normalized) uniform distribution is 0.29. What this mathematically means is that if one wants to treat the uniform randomization as a Gaussian counterpart, then he can use the term 0.29 to convert 1-D width to the RMS equivalent.

It is important to note that currently the Chandra on-axis PSF is dominated by the detector blurring effects due to the limited size of detector pixels, which is even slightly larger than the on-axis telescope PSF (FWHM). Typically, the PSF broadening due to pixelization is negligible only when pixel size is $\sim 1/2.5$ of FWHM.

### 4.5 Evaluation

One can roughly predict SER performance numerically from the PSF size in each stage. i.e., PSF after mirror, PSF after aspect blurring, and PSF after pixelization.

The PSF size at each stage can be roughly quantified by fitting the distribution to a 2-D Gaussian function. Before SER (without randomization), the CXO PSF is a convolution of the three individual parts, i.e.,

$$X = C_X + Rn(s, sz) \cdot A_{bf} + Ru(s, sz) - 0.5$$  \hspace{1cm} (4.4)
Figure 4.1: PSF scatter plot at different stages, i.e., after HRMA (left), HRMA + aspect blurring (middle), and after default ACIS pixelization (right). The simulations are at ACIS-S3, for photons with 1.74 keV, and 0''.07 aspect blurring factor.

\[ Y = C_Y + Rn(s, sz) \cdot A_{bf} + Ru(s, sz) - 0.5 \]  

(4.5)

Where \( C_X \) and \( C_Y \) are ChaRT simulated results in CXO Sky coordinate, after ChaRT and MARX simulations, for HRMA PSF distribution. \( Rn \) and \( Ru \) are pseudo-random number generator for normal uniform distribution, respectively. \( s \) is their seed value, and \( sz \) is the array size specifies how many random numbers should be generated. \( X \) and \( Y \) are values for \( X \) and \( Y \) direction in Sky coordinates. All the units are in (ACIS) pixels. \( Ru(s, sz) - 0.5 \) indicates that the standard ACIS pixel size is "one pixel", in square shape.

The PSF size at each stage can be calculated from figure 4.1, by forming a 2-D image of each panel, and fitting into a Gaussian function. The PSF sizes are 0.29, 0.427, and 0.625 arcsec for HRMA, telescope, and after standard ACIS pixelization (without randomization), respectively. Therefore, ideal SER removes pixelization effect completely and could change PSF from 0''.625 to 0''.427.
Chapter 5

Sub-pixel Event Repositioning
Algorithm for ACIS CCDs

5.1 Introduction

ACIS event grades classify how the charge was distributed. Even though there are as many as 256 different grades, events with charge distributed over more than 4 pixels are most probably formed by noise, like cosmic rays. In addition, charges split diagonally (like fitgrade 4, 36) or over a 3-pixel line (such as fitgrade 66, 24) are also most likely not generated by X-ray photons. Therefore, only 13 “viable” event grades are essential and can be divided into three subgroups: single pixel events, two-pixel split events and corner split events (see table 3.1). Among the 13 “viable” events, 12 are split events, and can be further divided into 3 split event subgroups: 2-pixel split events, 3-pixel split events, and 4-pixel split events. The last two (3- or 4- pixel split) subgroups compose corner split events. Those 13 ACIS fitgrades are “physically reasonable” grades and account for about 95% of all the events for a typical X-ray source. Other fitgrades are unrealistic and subject to rejection. The sub-pixel event repositioning (SER) algorithms for Chandra/ACIS imaging, the methods based on the premises that the charge cloud size is relatively smaller than
ACIS pixel and the impact position of events can be refined, based on the distribution of charge among affected CCD pixels, is to reassign the photon impact positions according to different event grades within the tolerance of uncertainty, with the intent to improve the already unprecedented angular resolution of Chandra X-ray imaging with the ACIS.

Standard ACIS images have spatial resolution limited by CCD pixel size, i.e., 24 microns or 0.492 arcseconds. In other words, the photon impact position has an uncertainty of a half pixel, 12 μm. However, as it is known that, only when photon impact locations are very close to the boundaries, split event grades can be formed. Therefore the PIP uncertainty is related to event grade. Different event types have different photon impact position (PIP) accuracy and uncertainty. For a photon with a certain energy, the generated charge cloud will have an average size proportional to its energy, and the shape can be well represented by a two dimensional axis-symmetric Gaussian function (Tsunemi et al. 1999b). If we assume the cloud radius is \( R_c \), then photon impact position (PIP) has to be around the cloud center within the range of \( \pm R_c \). This assumption is used for SER uncertainty analysis.

### 5.2 The Proposed SER Algorithm

When employed as the focal plane imaging array for CXO, ACIS collects incident X-ray photons in photon counting mode, which implicitly assumes that there is at most one photon in a \( 3 \times 3 \) subarray in one frame. ACIS registers individual incoming photons individually in an event list, which records spatial and spectral information, as well as the event grade. The grade indicates charge split morphology\(^\text{17}\) in an isolated \( 3 \times 3 \) pixel island centered at the event pixel (see section 3.4).

ACIS processing tools implemented by the Chandra X-ray Center (CXC) assume that all the events have same photon impact positions, i.e., at the event pixel center. However,

\(^{17}\)An ACIS keyword, FLTGRADE, gives the charge split morphology, i.e., how many and which neighboring pixels exceed a specified split threshold. Three groups of split events, i.e. 2-pixel, 3-pixel and 4-pixel split events, have different average shifts respectively, but we do not distinguish the difference for a given group in different directions. In other words, events with FLTGRADE of 11, 22, 104 and 208 all are 4-pixel split events but split to different corners; the absolute offsets are the same for those events.
as described in section 3.5, because the charge cloud size is very small compared with the ACIS CCD pixel size (Tsunemi et al. 1999a), the photon impact positions for split events will be close to the split boundaries instead of the pixel centers, offering the opportunity of subpixel event repositioning derived from the event charge distribution (grades). In addition, Chandra’s slow but intentional dither motion during a pointed observation moves the target across the detector surface (see section 3.4), in principle allowing full sampling of the PSF of the High Resolution Mirror Assembly, which otherwise would be sub-critically sampled by ACIS.

Tsunemi et al. (2001) have taken advantage of knowledge of X-ray event charge distribution among CCD pixel islands and the (subpixel) telescope pointing history, both of which are included as standard supporting data for a CXO observation, to first propose an SER algorithm for subpixel resolution improvement. Their SER model uses corner split events only, by assuming that, for 3- or 4-pixel split events, the actual photon impact positions are the split corners instead of the pixel centers. So the algorithm’s implementation consists of shifting events by one-half pixel along both pixel sides towards the split corner in Chip coordinates\(^{18}\), then projecting the new location into the Sky coordinates according to the chip orientation and the spacecraft roll angle. They also predicted that solely based on corner split events, the knowledge of photon impact position can be roughly improved by a factor of 10. They concluded that X-ray images constructed from repositioned corner split events only are almost free from degradation by the CCD pixel sampling.

However, there is a relatively small percentage of corner split events in a typical X-ray source, as listed in table 8.1, in which the branching ratio is calculated from Orion Nebula Cluster (ONC, Schulz et al. 2001) sources imaged by CXC/ACIS. Tsunemi et al. (2001) and Kastner et al. (2002b) also note that corner split events only constitute about 4% to 16% of total events, depending on the source spectrum and CCD type employed. Thus the

\(^{18}\)There are three fundamental coordinate systems in CXO event list, i.e., Chip coordinates, Detector coordinates and Sky coordinates. The conversion among them is unique. Refer to McDowell (2001) for detail.
improvement of spatial resolution of their original SER is at the cost of low efficiency and suffers for faint sources. In addition, since the PSF of the telescope (including HRMA psf and aspect blurring) limits the spatial resolution, the spatial resolution of Chandra would reach its maximum, i.e., be telescope limited, so long as we critically oversample the PSF, e.g., sampling at \(\sim 0''.25\).

Mori et al. (2001) modified the Tsunemi et al. (2001) SER method by adding 2-pixel split events and single pixel events, in order to improve the statistics. Both the Tsunemi et al. and Mori et al. methods assume that all the corner split events take place precisely at the split pixel corners, while 2-pixel split events occur exactly at the centers of split boundaries. Physical CCD models (Prigozhin et al. 2002) have demonstrated that corner split events can be formed even for photon landing somewhat far from the corners, where the distance is a function of photon energy. These simulations indicate that the assumed landing positions of split events can be refined via a reliable physical model of the CCD-photon interaction.

5.3 SER Modification: Expanding Event Selection Criteria

To overcome small number problems and thereby improve the capability on faint sources of the SER method proposed by Tsunemi et al (2001), it is reasonable to use all 13 “viable” event grades. As demonstrated later, 2-pixel split events have better position accuracy in one direction, and account for a big percentage of all event grades, while one pixel events account for a large fraction of a source count, and have PIP uncertainty smaller than a pixel (Kastner et al. 2002b). Upon analysis of the ACIS simulations (see section 6.2), we found that most single event landing positions are near the pixel centers, and constrained in an area slightly smaller than an ACIS pixel. Two-pixel split events are generated by photons that land near the center of split boundaries, and are limited to a “quadratic curvature” area, while the landing positions of corner split events are limited to the smallest area, close to the split corners, with a cometary shape. Because the charge cloud size is very small compared with ACIS pixel size, single-pixel events will have the biggest position uncertainty.
in both directions along pixel sides, and corner split events have the smallest uncertainty among all the events in both directions, while 2-pixel split events have smaller uncertainty in the direction perpendicular to split boundary, and have larger uncertainty in the direction parallel to split boundary.

Therefore, in the implementation of SER, the Tsunemi et al. (2001) model has been modified by adding 2-pixel split events and single pixel events. It was assumed that corner split events take place at the split corners instead of event pixel centers (as also assumed by Tsunemi et al. 2001), and 2-pixel split events occur at the centers of split boundaries, 0.366 and 0.47 pixels away from the pixel centers (see section 5.3.2), for BI and FI CCD respectively. Single pixel event PIPs remain at the event pixel centers, as there is no way to refine these PIPs based on charge distribution. The 0.366-pixel offset for 2-pixel split events in BI devices was determined empirically by trials on Orion BI CCD data, while the FI 0.47-pixel offset is determined from high fidelity FI CCD model simulations\(^\text{19}\). This modified algorithm is hereafter referred to as “static” (or “energy-independent”) SER. The algorithm's schematics can be found in figure 5.6, in which the pixel island and assumed photon impact positions are displayed.

In order to implement the static SER algorithm and understand the potential improvement of applying this algorithm, the three subgroups of the “viable” events will be briefly discussed in the following sections, as well as their location uncertainties.

### 5.3.1 Single Pixel Events

Single pixel events (grade 0) are those whose charge deposition is confined within one pixel. Photons absorbed near the pixel center will likely deposit all the electron charge in one pixel. Even though there is no way to improve on PIPs for single events according to charge distribution morphology, these events are included because: (1) they account for a large

\(^{19}\)0.366-pixel offset for 2-pixel split event at BI devices was determined from BI ONC data, and the result is consistent with the later BI ACIS simulations. This offset was tested on FI ONC data too, and found has better improvement than half pixel shift. Later FI CCD model simulations show that 0.47 pixels is the best offset for FI 2-pixel split events.
amount of the total events, especially for FI data (see table 8.1); (2) the uncertainties in photon impact locations are smaller than a pixel size, especially for BI CCDs.

Since the charge cloud is much smaller than the pixel size, single pixel events have the greatest uncertainty among all the acceptable events.

Figure 5.1: Single pixel event photon impact position distribution. Results are from MIT BI ACIS model (see 6.2), and simulated photons have monochromatic energy of 1.74 keV.

Figure 5.1 shows the photon impact position distribution for single pixel events. Simulated photons have monochromatic energy of 1.74 keV. The function can be estimated by a Gaussian function, and indicates the uncertainty of the landing positions. The figure indicates the relationship between PIP and the possibility of forming single-pixel events. The function itself also indicates the PIP uncertainty, i.e., the fatter the shape is, the larger the uncertainty. The FWHM (therefore uncertainty) of this Gaussian function actually depends on the photon energy and photon interaction location. Because higher photon
energy events form larger charge clouds, the possible PIP has to be in a smaller region for single high-energy events. In other words, if a photon was absorbed deeper, the charge has larger diffusion time, thereby the collected charge cloud is bigger, and the PIP uncertainty is smaller.

Figure 5.2 schematically shows the SER assumed photon impact location and its uncertainty for single pixel events. Assuming the collected charge cloud has a Gaussian shape with radius $R_c$ (radius can be defined as $\sigma$ or $\frac{1}{2}$FWHM), the possible photon impact position can be anywhere within a square\footnote{Strictly, the shape is irregular (see figure 6.4 and 6.7). Because a pixel is physically square shaped, the author approximates the uncertainty region as a square to simplify analysis. Same rule holds for 2-pixel and corner split event PIPs.} $(24-2R_c) \times (24-2R_c)$ centered at pixel center, in units of $\mu$m. Therefore, the uncertainty of the single event PIP is $\frac{1}{2}(24-2R_c)\mu$m in both directions, instead of one half pixel.

### 5.3.2 Two Pixel Split Events

Charge collected in two up-down or left-right adjacent pixels are 2-pixel split events (excluding diagonal), in which the photon impact positions are close to the centers of the split
boundaries. However, the best offset for 2-pixel split events is not one half pixels, but 0.366 and 0.47 pixels away from the pixel centers towards split boundaries instead, for BI and FI devices, respectively.

The 0.366-pixel offset for BI devices was experimentally determined by minimizing the FWHM of a point source in on-orbit ACIS-S3 BI CCD data (Schulz et al. 2001). The source has a good shape that can be well represented by a Gaussian function, with enough counts to ensure statistical accuracy. The source information was listed in table 8.3 (source # 6), i.e., 15.1 away from optical axis, with photon count rate of 0.077 counts per second.

In order to determine the best offsets for 2-pixel split events, the size (FWHM) of the chosen source was measured after applying SER correction, in which the offset of 2-pixel events varies, and corner-split events are assumed at split corners. After event position correction, all the events were used to create the intensity image in Sky Coordinates, then performed 2D Gaussian fitting. FWHM of the source was calculated from the fitted Gaussian function. Figure 5.3 shows source FWHM variation in terms of 2-pixel split events offsets, and indicates that an offset between 0.36 and 0.37 pixels can minimize source size. Analysis of other point sources shows that 0.366-pixel offset is the best.

The experimental outcome was adopted for the modified BI SER to correct PIPs for 2-pixel split events. In addition, this result is consistent with the output of later BI CCD model simulations. The FI offset, 0.47 pixels, however, is directly determined from high fidelity FI CCD model (Prigozhin et al. 1998b) simulations, for soft (less than 4 keV) X-ray beams (see figure 6.9). Applications on Chandra/ACIS observations show better improvement by applying 0.366- or 0.47-pixel shift for 2-pixel split event than that by one half pixels shift, which as assumed by Mori et al. (2001).

By assuming charge cloud radius as $R_c$, the possible interaction location is confined to a rectangle, with size of $24 - 2R_c$ in the direction parallel to split boundary, and of $2R_c$ perpendicular to the split boundary. The small area is centered at 0.366- and 0.47-pixel away from the pixel center, for BI and FI CCDs, respectively. Refer to figures 5.4 and 5.6
Figure 5.3: The source FWHM variation in terms of changing 2-pixel split event offsets. Points with “plus” symbols stand for source sizes after SER correction, but at different offset for 2-pixel split events. “Circle” symbols indicate original source size without SER correction but after removing randomization.

for schematic illustration.

The PIP offset for BI and FI devices has to be differentiated, because ACIS BI and FI devices are different in thickness, structure, and “dead layers”, as well as the surface that incident photon strikes. The collection of signal charge occurs near the front surface, the same one that is illuminated by the incoming photons in the FI CCD. Much larger fraction of photons interact close to the surface of the device where electric potentials are influenced by the grounded channel-stop layer, resulting in a very different charge splitting pattern compared to the one in the BI devices. On average charge clouds are formed closer to the collecting potential wells and travel shorter distances, therefore having less time to expand. Smaller charge clouds reduce the possibility of forming split events.

A thicker dead layer covering vertical charge-splitting pixel boundaries of FI CCD is another factor contributing to reduction of the share of split events. As a result Tsunemi
et al. (2001) SER technique for FI devices suffers seriously from low detection efficiency.

Figure 5.4: Schematic diagram of 2-pixel (left) split event (fltgrade 2), with the ACIS assumed landing position, new assigned location, and PIP uncertainty.

Compared to a single pixel event, the PIP distribution of a 2-pixel split event has a different shape and a smaller size. Since there are 4 different grades for 2-pixel split events, the region to which the PIP is confined depends on the charge split direction. For a left-split event (fltgrade 2), for example, the specific PIP region is (approximately) a rectangle, centered at split boundary, 0.366 pixels away from the pixel center, as shown in figure 5.4. The photon impact position distribution of 2-pixel split event is actually an axis-symmetric Gaussian function. The FWHM of the Gaussian function will be slightly different for up-down split event with left-right split event, because of the dissimilarity between the up-down boundary and left-right boundary — vertical (up-down) boundaries are formed by low-state gates while the horizontal (left-right) boundaries are formed by p+ doped channel stops. The physical properties and statistics are also different for the two different boundaries. However, perhaps because the difference is minor, neither simulation data nor observations show the apparent discrepancy. Therefore, we can approximate that, by assuming collect charge cloud has a size of $R_c$, the PIP is confined to a rectangular region centered 0.366 pixels away from event pixel center towards split boundary, with the size of $2R_c \times (24-2R_c)$. The orientation depends on the event grade. In other words, the uncertainty for 2-pixel split
event is \( Rc \) in one direction, and \( \frac{1}{2}(24-2Rc) \) in the other direction, instead of the half-pixel uncertainty defined by standard ACIS event processing.

### 5.3.3 Corner Split Events

The 3- or 4-pixel corner split events\(^{21}\), formed by photons which were absorbed near the pixel corners, have the smallest photon landing uncertainties among the various event subgroups. Therefore, corner split events have the most accurate landing locations among all the events. The PIP distribution of those events can be approximated by a Gaussian shape — whether circularly symmetric or axial symmetric is unknown, again, because of different physical properties of the two boundaries — and is assumed to be centered at the split pixel corner. Without loss of generality, one can assume the Gaussian shape is circularly symmetric with size \( Rc \). Consequently, the PIP is confined to a region which is approximately a square, centered at the split corner, with the size of \( 2Rc \times 2Rc \). So the uncertainty of corner event impact position is \( Rc \) in both horizontal and vertical directions instead of half-pixel as defined by ACIS. See figure 5.5 for a schematic illustration.

However, later simulations from CCD models show that assuming PIPs for corner split events lie at split corners is not accurate, especially for BI 3-pixel split events. Nevertheless, here Tsunemi et al. (2001) method was adapted, in which corner split events were assumed to have PIPs at split corners.

### 5.3.4 The Modified SER Algorithm

According to above analysis and assumptions, this static SER (SSER) algorithm reassigns photon impact locations on Chip coordinates only depending on event grades. Then the new locations were projected back to Sky coordinates to reconstruct the object. The schematic diagram (figure 5.6) shows the SER algorithm reassigning PIPs for different events on a 3 \( \times \) 3 pixel island (not to scale) displayed at Chip coordinates, where the central pixel is

\(^{21}\)In this document Corner event, corner split event, and 3- or 4-pixel split event are interchangeable. These events deposit charge in 3 ("L" shape) or 4 (square shape) adjacent pixels.
Figure 5.5: Schematic diagram for corner (upper-left, fitgrade 72 or 104) split event and its photon impact locations with and without SER assumption.

event pixel, and the pixel center is ACIS presumed landing location (marked by a five-point star). Solid circles represent SER reassigned photon impact locations, according to the event subgroups, while the shaded areas are the possible photon impact areas for different event subgroups. The detailed algorithm implementation and examples are described in section 5.4 and 5.5.

5.4 The Algorithm Implementation

The basic implementation of the algorithm is as follows: depending on the event's flight grade, reassign the photon’s impact position from the default location (pixel center) to the inferred location in Chip coordinates. Then according to CCD chip orientation, as well as the telescope pointing and spacecraft roll angle history of the observation, convert the new
Figure 5.6: Schematic illustration of the subpixel event repositioning algorithm, after expanding event selection criteria.

Chip location to Detector coordinates and, finally project to Sky coordinates.

As described in above sections of this chapter, the subpixel event repositioning algorithm is mathematically simple in principle. However, because of the complexity of Chandra, ACIS, and their coordinate systems, the implementation of the algorithm requires some care.

In order to analyze the detected event and to track back where the photon originates on the Sky, three fundamental coordinate systems were defined for convenience. The Chip coordinate system, which records photon position in the CCD (chip) plane, assumes that each chip is a perfect plane with uniform pixel size. The Detector coordinate system, or the focal plane coordinates, records the photon positions in the tangent plane of the optical axis. The Sky coordinate system, which is a perpendicular space to a nominal fixed celestial pointing direction, locates photons in such a fictitious tangent plane (McDowell 2001).

There is a unique but complicated procedure to convert a photon position from Chip to Detector to Sky coordinates, and vice versa. Because the ten ACIS chips are slightly tilted to
maximally approximate the telescope's focal surface, not all the chips are parallel to detector coordinate plane, and each one has its own location and orientation on the "optical bench" (McDowell 2001). Therefore converting Chip coordinates to Detector coordinates has to take account of other considerations, like local science instrument (LSI), SIM translation table (STF), SIM translation frame (STF), etc. In brief, the conversion goes through the following steps,

CHIP: CPC $\rightarrow$ LSI $\rightarrow$ STT $\rightarrow$ STF $\rightarrow$ FC $\rightarrow$ MNC

where the meaning of each abbreviation can be found in table 5.1. Interested readers may refer to McDowell (2001) for detailed information.

The subpixel event repositioning algorithm reassigns the photon impact position at Chip coordinates, then projects the new location to Sky coordinates (via Detector coordinates) to reconstruct the X-ray sources. However, as already described, the PIP shift is very small (less than one half ACIS pixel in each direction in Chip coordinates). In order to simplify the algorithm and minimize the calculation time, the algorithm simply assumes that the shift in Chip coordinates equals to the shift in Detector coordinates, and absorbs the chip orientation/tilt errors into off-axis angle, similar to that Chandra PSF absorbs the mirror shell differences for different energy photons. The error due to this simplification is fairly small comparing to PIP uncertainties even for corner split events. Future modification of SER algorithms might release this simplification, for the purpose of the finer angular resolution improvement.

Figure 5.7 shows the orientation of each ACIS chip when projected to Detector coordinates. The pixel orientation that was used in this thesis is described in figure 5.7 too. For a split event, it is necessary to know the split direction in order to reposition the photon landing location. So a corner split event has four possible split directions referred as LL, LR, UL and UR, respectively (refer to table 5.1). A two pixel split event also has four possible split directions, i.e., up, down, left, and right split. The flight grade of an event indicates whether the event is split, and, if yes, the split direction.
Figure 5.7: Orientation of each ACIS chips in Detector coordinate definition.

The first step of SER implementation is to relocate the photon impact positions in Chip coordinates, according to the events' \texttt{FLTGRADE}\textsuperscript{22}. Remember that ACIS automatically assigns the PIPs at the event pixel centers. However, for example, events with grade 104, which means UL corner split, have PIPs close to UL corners of the event pixels. Therefore SER methods move PIPs into the new locations by changing their Chip coordinates.

The second step is to calculate the new location in Detector coordinates. Here, it is simply assumed that all the ACIS chips are in one plane and parallel to (tangent) Detector plane. This assumption is not true actually, as mentioned before, and can only be closely

\textsuperscript{22}ACIS instrument keyword, means flight grade, in order to differentiate ASCA keyword GRADE. But in this literature, as mentioned before, both fitgrade and grade implicitly refer to ACIS flight grade, except explicitly stated.
approximated for near on-axis sources. However, the approximation errors can be absorbed into the off-axis angle parameter. This assumption means that the shift of PIPs in Chip coordinates have the exactly same amount as the shift of PIPs in Detector coordinates, thus simplifying the calculation.

Figure 5.7 shows that different ACIS chips have different (but fixed) orientations respect to Detector coordinates. Therefore, when the PIP shift in Chip coordinates is converted to Detector coordinates, the employed ACIS CCD chip where the event took place needs to be determined. This is facilitated by use of the event list column giving information of the CCD identification number (tag name CCD.ID), which specifies individual CCD chips (table 5.2).

If "M" is defined as the transform matrix of the amount of rearrangement from Chip to Detector coordinate, then there are three different \( \text{Ms} \) according to different CCD chips. Equation 5.1 lists those rotation matrices for different CCD chips.

\[
M = \begin{cases} 
\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & \text{if CCD is } I0, I2 \\
\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & \text{if CCD is } S0, S1, S2, S3, S4, S5 \\
\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} & \text{if CCD is } I1, I3 
\end{cases} 
\]  

(5.1)

The third step of implementing SER is to project the PIP shifts in Detector plane to Sky coordinates. By default, the two planes are parallel to each other, and have exactly same pixel size with unit of arcsecond. However, the axis in detector coordinate is in principle of right hand, meaning x-axis increases rightward, while y-axis increases upward. But the Sky coordinate is related to the World coordinates, and the spacecraft is in the inside of the celestial sphere looking out, so the right ascension increases to the left. Therefore,

\[-\Delta X = \Delta Y = \Delta \]  

(5.2)
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPC</td>
<td>Chip Physical Coordinates</td>
</tr>
<tr>
<td>LSI</td>
<td>Local Science Instrument</td>
</tr>
<tr>
<td>STT</td>
<td>SIM Translation Table – Optical bench</td>
</tr>
<tr>
<td>STF</td>
<td>SIM Translation Frame – Instrument module</td>
</tr>
<tr>
<td>FC</td>
<td>Focal Coordinates</td>
</tr>
<tr>
<td>MNC</td>
<td>Mirror Nodal Coordinates</td>
</tr>
<tr>
<td>DET</td>
<td>Detector (focal plane pixel) Coordinates</td>
</tr>
<tr>
<td>TDET</td>
<td>Tilted Detector Coordinates</td>
</tr>
<tr>
<td>LL</td>
<td>Lower Left</td>
</tr>
<tr>
<td>LR</td>
<td>Lower Right</td>
</tr>
<tr>
<td>UL</td>
<td>Upper Left</td>
</tr>
<tr>
<td>UR</td>
<td>Upper Right</td>
</tr>
</tbody>
</table>

Table 5.1: Coordinate abbreviations

<table>
<thead>
<tr>
<th>CCD-ID</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>CCD Chip</td>
<td>I0</td>
<td>I1</td>
<td>I2</td>
<td>I3</td>
<td>S0</td>
<td>S1</td>
<td>S2</td>
<td>S3</td>
<td>S4</td>
<td>S5</td>
</tr>
</tbody>
</table>

Table 5.2: ACIS CCD IDs and corresponding chips.
The roll angle of the spacecraft is the rotation angle of the two parallel plane (Sky and Detector), and named as $\gamma$. So the transform of the displacement in Detector plane to Sky plane is:

\[
\begin{bmatrix}
-\Delta Sky X \\
\Delta Sky Y
\end{bmatrix} = \begin{bmatrix}
cos\gamma & -sin\gamma \\
\sin\gamma & \cos\gamma
\end{bmatrix} \begin{bmatrix}
-\Delta Det X \\
\Delta Det Y
\end{bmatrix} \quad \text{or} \quad (5.3)
\]

\[
\begin{bmatrix}
\Delta Sky X \\
\Delta Sky Y
\end{bmatrix} = \begin{bmatrix}
cos\gamma & \sin\gamma \\
-sin\gamma & \cos\gamma
\end{bmatrix} \begin{bmatrix}
\Delta Det X \\
\Delta Det Y
\end{bmatrix} \quad \text{(5.4)}
\]

The refined Sky coordinates then can be used to reconstruct the image. Comparing with the original image, the improvement of subpixel event repositioning algorithms can be evaluated. The working regime of the SER algorithms and their applications will be discussed in later chapters.

### 5.5 Static SER: an Example

Figure 5.8 shows an example before and after applying the static SER algorithm. The source (source No. 10 in table 8.3) is from Orion Nebula Cluster (Schulz et al. 2001), observed in November 1999 by Chandra using ACIS S3 back-illuminated CCD detector. The source has an off-axis angle of 11.56 arcseconds, with total event count of 1420 photons. Among them 378 counts are corner-split events, or 26.6% of all events, the 2-pixel split event percentage is 48.7%, and the single pixel event percentage is 19.9%. Thus the split event percentage is 75.4% of all the events, and the percentage of source events used in the SER algorithm is 95.2%. So the rejected events constitute 4.8% of all the detected counts. Only 3- and 4-pixel split events were used in figure 5.8. The left panel is the raw level 1 Chandra data (after removing randomization), in which the photons are loosely distributed. The right panel is after applying the static algorithm on the data from the left panel. One can see that the photons were in general brought closer to pixel center, and the source is more compact.
Figure 5.8: Corner split events layout of a point source in BI ONC observation (ObsID 04). Left: The event locations after removing randomization but before applying Static SER. Right: The event locations after removing the randomization and applying static SER algorithm. 4 colors in the plot stand for 4 sub-groups of the corner split events: Lower Left split, Red; Lower Right split, Green; Upper Left split, Blue; Upper Right split, Magenta. The plots are in Sky coordinates, and dotted box stands for an area of 8 × 8 pixels. Small dashed boxes stand for one pixel in Chip coordinates, and the orientation indicates telescope’s roll angle.
Figure 5.9: Reconstructed image before and after applying event repositioning for the same ONC source displayed in fig. 5.8. The pixel size is half of ACIS’ intrinsic size, and contour curves are from Gaussian smoothed image (kernel with FWHM=0".5). The levels are 15, 30, 45, 60, 75, 90 percent of the peak value of the event repositioned image. Left: Reconstructed image before event repositioning, i.e., event filtered raw Chandra image without randomization. Right: Event repositioning algorithm applied on the left image. The pseudo color in the plots stands for source intensity. The maximum value plotted in the two panels is same.

Figure 5.9 shows the reconstructed ONC source displayed in figure 5.8 before and after applying static SER method. However, the images were constructed not only from corner pixel split events, but also from single pixel events, and two pixel split events. The images have contour levels overplotted. Note that the pixel size was binned down to half of the ACIS intrinsic pixel size, i.e., 0".25 in the image. Two-dimensional Gaussian fitting function was used to fit the image’s intensity and to estimate the improvement. The FWHM of the fitted Gaussian function is 1".03 before event repositioning, and 0".82 after. The improvement in spatial resolution is 60.8% if we measure improvement (following from Tsunemi et al. 2001) as

\[ \Delta = \sqrt{F_B^2 - F_A^2} / F_B \]  \hspace{1cm} (5.5)

where \( \Delta \) is the improvement, \( F_B \) and \( F_A \) are the FWHMs of the 2-D Gaussian fitted image before and after applying SER algorithm, respectively.
5.6 Other Possible Parameters

In the static (energy-independent) model, event grade and CCD type are the only parameters to determine photon impact positions. However, there are a few other parameters that might affect the uncertainty besides event grades, like photon energy, charge split fraction in the split pixels, even CCD working condition, charge transfer inefficiency, and charge loss, to improve PIP uncertainty. Some of those parameters might be significant and worthy of further exploration, to improve the SER performance.

It is already clear (section 5.3.2) that static SER can be divided into FI SER and BI SER methods, because of the differences between BI and FI devices. Empirical results reveal that the cloud size is relatively smaller for FI CCDs than in BI ones, for photons with the same energy. So the average offset for a subgroup of split events is different than those concluded from BI devices. In addition, because of the low split event percentage, the improvement after applying SER to FI data may be less than that for BI data.

**Photon energy:** Photon energy is a very important parameter in the subpixel event repositioning algorithm. First, photon energy determines the initial charge cloud size, and finally affects the collected charge cloud size. Second, photon energy directly relates to photon absorption length in silicon, which statistically delimits where the photoelectric interaction takes place. The photon absorption location determines charge diffusion time before it reaches the collection gates, which directly relates to charge cloud radial expansion. Therefore, photon energy eventually dictates the collected charge cloud size, and hence the photon impact position uncertainty. Further modification of the SER algorithm will be energy dependent in order to achieve better spatial resolution. Based on the multi-pitch mesh experiment on an X-ray CCD, Tsunemi et al. (1999b) determined that the charge cloud size monotonously increases as photon absorption length increases. The right panel in figure 3.7 shows the relationship between photon attenuation length in Silicon and the

---

23Note the difference between three subgroups of events and three subgroup of split events. The three subgroups of events mean single pixel events, 2-pixel split events, and corner (including 3- and 4-) split events. The three subgroups of split events represent 2-; 3- and 4-pixel split events.
measured charge cloud size by multi-pitch mesh experiment. The results in both horizontal and vertical directions are shown there, and indicate the discrepancy between the X and Y direction boundaries, for the CCD they used in the experiment. Note that this result is from the experiment setup for their specific front-illuminated CCD (12 μm pixel size) and its operating condition (25 μm depletion region). However, because ACIS CCD has different physical properties and operation conditions, the outcome will be different. In addition, two ACIS-S CCDs are back-illuminated, and on-orbit operating conditions ensure the two BI CCDs are fully depleted.

**Charge split proportion:** Other than the event grade, which tells how the charge split and near which boundary the photon probably landed, the charge split fraction among adjacent pixels may indicate how far the PIP is from the split boundary. Intuitively, for a split event, a larger charge proportion in a split pixel means the PIP is closer to the split boundary, and vice versa. Therefore, by including information concerning charge split proportion, the PIP accuracy must be improved.

This parameter should be more fruitful for BI devices, since the landing area for photons leading to split events is much bigger than for FI devices. Therefore including this parameter could reduce the PIP uncertainty. For FI devices, because of the larger depletion region, only those photons that interacted very close to boundaries can result in split events. Therefore, including charge split proportion information might be not so significant for FI devices.

**CCD operating conditions:** CCD operating conditions, such as temperature, applied gate voltage, etc., determine the thermal noise, charge transfer inefficiency (CTI) and depletion region depth. The thermal noise and CTI will affect energy resolution, split event recognition, and effectively redistribute event grades. The depth of depletion region influences charge collection efficiency (CCE), as well as collected charge cloud size, and eventually affects branching ratio. However, those factors are regularized and normally immutable on orbit.

**Charge loss:** Charge loss, a subtopic of CCE, takes place when the photon was
absorbed in the "dead layers" — such as gates or channel stops. In addition, it will happen during the charge diffusion period if photon absorption occurs in the field free region. A very small amount of charge will be lost also during readout time because of the charge transfer inefficiency, but this is negligible compared to the first two mechanisms. Charge loss definitely affects energy resolution, it also influences split event differentiation, and eventually affects the SER algorithm.
Chapter 6

Further Modifications from
Existing ACIS CCD Models

Several simulators for Chandra and/or ACIS are currently available. The most widely used one is Model of AXAF Response to X-rays which was designed and created by CXC group at MIT (Massachusetts Institute of Technology). This program suite can run in sequence to simulate Chandra on-orbit performance, with FITS\(^{24}\) file and image output. All kinds of built-in instrument models, including HRMA and focal plane detectors, enable MARX to perform a ray-trace and thereby simulate how Chandra responds to a variety of astrophysical sources. Post-processing routines can simulate aspect movement and ACIS photon pile up. Other auxiliary tools make FITS image file or event list output possible.

However, ACIS simulations in later MARX versions have less capability to take full advantage of the subpixel resolution that was offered by Chandra/ACIS imaging. Therefore, SER related simulations have to rely on specialized ACIS CCD simulators, to analyze the charge distribution, grade formation, and SER implementation as well. Two ACIS simulators are available so far, one created by scientists at Pennsylvania State University

\(^{24}\text{FITS}:\) Flexible Image Transport System. FITS data format is the standard astronomical data format endorsed by both NASA and the IAU. FITS is much more than an image format (such as JAG or GIG) and is primarily designed to store scientific data sets consisting of multi-dimensional arrays (1-D spectra, 2-D images or 3-D data cubes) and 2-dimensional tables containing rows and columns of data. [?]
(PSU), and the other built by MIT researchers.

6.1 MARX and PSU ACIS Simulator

The PSU CCD simulator, which was developed mainly by Leisa Townsley and Patrick Broos in Penn State University, is a Monte Carlo Method for simulating X-ray CCDs. The simulator is for characterizing and calibrating the ACIS instrument designed in CXC. It contains machinery for simulating both BI and FI X-ray CCDs. This simulator was developed to combine with early version of MARX simulation output.

The simulator can be used jointly with MARX simulation, to predict Chandra/ACIS imaging functions. When simulating MARX with ideal detectors, the simulator takes the raw binary outputs as its input, and tracks the grazing photons until they interact with (or penetrate through) the CCD.

The simulator can reproduce the detected CCD event spectrum, the quantum efficiency, and event grade distribution. The model relies on a charge distribution equation to predict charge radial distribution on CCD field free region. In order to simulate sub-pixel structure of a real CCD, the simulator includes a built in model of channel stop and isolation layer underneath the gate structure.

As mentioned earlier, PSU ACIS simulator was developed in the early days of MARX, and is not well updated. MARX has been modified many times, to keep as close as possible to current on-orbit CXO performance. Some MARX parameters and outputs have been changed, with the up-to-date calibrated data. Therefore, the simulator is not very suitable for direct use with later published MARX versions.

However, this ACIS simulator can still be used to investigate the event-repositioning algorithm by specifying photon landing positions for a given energy. This was done by manually changing MARX raw binary output, like the photon interactive location and detected energy. The result shows that when a photon lands near a pixel center, it most probably will form a single event, whereas when a photon lands near a pixel boundary, it
has a high chance to generate a split event. This phenomenon confirmed that the event relocation algorithm is feasible. A few outputs of the combined simulation (MARX + PSU ACIS) are presented here.

![Graphs showing split event probability](image)

**Figure 6.1:** The grade analysis of 1.775 keV photons for PSU BI CCD simulator. The lines with “plus” signs in this and next three figures represent the simulated data, while the dash-dotted lines represents a Gaussian fit to the data. Dotted line at 0 μm represents the pixel boundary. The small boxes in the upper right corner of each panel stand for ACIS pixels, where the solid lines are the boundaries. The dotted line indicated the orientations of the displayed photon impact positions.

Figure 6.1 illustrates the simulation results for charge split fraction versus photon impact positions within an ACIS S3 pixel. The simulated monochromatic photons have
energies of 1.775 keV. The abscissae in the plots are the distance of photon landing locations away from the pixel boundary, horizontally or vertically. The small boxes in the upper right corner of each panel represent ACIS pixels, in which the solid lines stand for the pixel boundaries, while the dotted line stands for track of photon impact positions that is displayed along the x-axes.

By specifying the X-ray photon beam landing positions inside a pixel, the PSU simulator simulates the photon interaction and charge collection according to its own model, and forms an event grade to indicate charge split direction. The upper left panel is horizontal splitting simulation, while the upper right panel is the vertical splitting simulation. The figure shows that the two upper panels are very similar, indicating that vertical or horizontal split at this energy is quite similar for this BI CCD model.

The lower two panels are corner split fraction simulations. The photon landing locations in the left one are on UL-LR diagonal, while in the right panel are on LL-UR diagonal. Note that the abscissa axes in the plots represent the distance from pixel boundary (either horizontal or vertical, since they are same), not from a corner, while the y-axes stand for the corner split event fraction.

Also note that the two parallel boundaries (and two diagonal-opposite corners) in a pixel are not distinguished. The upper left panel in figure 6.1, for example, shows the horizontal 2-pixel split fraction when photon impact positions cross the line as shown in the upper right corner. When a photon lands near the left boundary, either grade 8 (left split) or 16 (right split) can be formed. So the plot in this panel actually shows the sum of left-split and right-split fractions. Similarly, the plot in the upper right panel shows the sum of up-split and down-split fractions, and the plots in the lower panels illustrate the sum of all "reasonable" 3- or 4-pixel split event fraction. The plots in the following three figures have the same symbols and explanations.

Figures 6.1 to 6.3 also show that not all the split events occur only when photons land on or very close to the split boundaries, such as corner split events that can happen
Figure 6.2: Flight grade distribution versus subpixel photon landing distances from a boundary for ACIS-I2 (FI) PSU CCD simulator. The photons have an energy of 1.775 keV. Symbols of each panel are as in the previous figure.
Figure 6.3: Flight grade distribution along the photon impact locations within a pixel by 3.0 keV photons for PSU ACIS CCD model. Symbols of each panel are as in the previous figures. Up 4 panels: ACIS-S3 (BI); Low 4 panels: ACIS-I2 (FI).
when photons interact as far as a few microns away from the split corners. In addition, the photon interaction distance for split events are energy and device type dependent. This fact indicates that SER algorithm can add the device type and photon energy as parameters, to offer better performance.

Further simulating of Chandra/ACIS observations using MARX and PSU ACIS simulator wasn’t performed, due to aforementioned considerations. Instead, the proposed simulations, including point-like sources with different intensity, spectrum and off-axis location, were carried out with the MIT CCD simulator, using MARX* simulation output. The purpose of those simulations is to fully explore the SER performance, and compare the SER results from real CXO observations. In addition, the binary system simulations were accomplished too, to demonstrate SER ability to distinguish binary objects.

6.2 The MIT CCD Simulator

The MIT ACIS simulator is a Monte Carlo model of ACIS CCDs (CCID-17, Prigozhin et al. 2002), and has two versions, one for backside-illuminated (BI) CCDs, one for frontside illuminated (FI) devices. The simulator can only be used for monochromatic simulations at each simulation; in default, the code itself randomly (uniformly) generates photon impact positions with subpixel accuracy and simulates where the electron clouds were formed and how the charge was spread across the pixels. Later modifications added an argument that specifies the subpixel photon impact position, for the purpose of SER simulation (combining with MARX). The output of the simulation includes subpixel photon impact locations and the signal amplitude in the pixels of the 3 × 3 pixel island, as long with the detect photon energy. Thus the simulation with this CCD model enables one to analyze how the charge was split, when photon impact positions vary within a pixel.

The simulator models can be used for many SER related analysis, such as to assist analytical SER performance prediction. Hereafter, this simulator is implicitly referred wherever the simulator (or CCD model) is mentioned, unless explicitly stated otherwise.
This simulator provides a convenient way to analyze event formation regulation at different (monochromatic) photon energies. It is also helpful to answer questions such as: What is the average PIP distance (relative to a pixel boundary) of each event subgroup (like single events, 2-, 3- or 4-pixel split events)? What is the function of charge percentage in the split pixel(s) relative to the distance between PIPs and the split boundaries for each event group? What is the performance difference between the BI and FI CCD devices?

Figure 6.4: The landing locations of different split event grades for photons with energy of 1.74 keV. Results are from MIT BI CCD model. Note that the axes are in the unit of pixels.
6.3 Energy Dependent SER

Figure 6.4 shows a simulation results from the BI MIT ACIS model. The simulation is carried out on a standard on-orbit ACIS-S3 (BI CCD) condition (like temperature, noise level, gain, etc.), for photons with energy of 1740 eV. The figure shows all 13 “viable” events PIPs within a pixel, and indicates that although each event type has its own PIP “territory”, these territories slightly overlap each other. This shows that, within a certain small area of a pixel, all three kinds of (subgroup) events could be generated. Furthermore, the size of the area that produces specific event charge split pattern changes according to photon energy. Therefore, the critical question for further SER modification is how best to determine the shifts for the split events.

Figure 6.4 is the monochromatic photon simulation, which implies that not all corner split events take place at the pixel corners, nor the 2-pixel split events occur at the center of split boundaries. Instead, the photon impact locations of split events are somewhat far away from the split boundaries, as well as energy-dependent, thus indicating the possibility of improving angular resolution by the SER algorithm, and further improvement by taking account of photon energy.

The high fidelity simulators can be used to build a table to determine the best shifts for each split event subgroups, according to photon energy, to modify SER as energy dependent. The simulations performed to date consist of 10,000 photons at each energy from 300 eV to 12 keV, with an energy step of 100 eV, on both BI and FI devices. Because of the attenuation-length jump around 1800 eV, the energy step was lowered to 10 eV from 1800 eV to 1900 eV. For each simulation, the branching ratio was calculated for single pixel events, 2-pixel split events, and corner split events; and the average subpixel position shifts for 2-, 3-, and 4-pixel split events. The BI simulated results are shown in figures 6.5 and 6.6.

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25Because of the small QE for FI devices at lower energy, the number of simulated photons at lower energy was increased to improve statistic accuracy.
Figure 6.5: Split event fraction vs. energy. The fractions of different event grades (branching ratio) vs. photon energies, with the X-ray attenuation length in silicon overplotted. Note that the attenuation length is in unit of 50 microns.
Figure 6.6: BI energy-dependent SER shifts vs. energy. The mean shifts from pixel centers of the three subgroups of split events, according to the photon energy.
Figure 6.5 shows the event percentage as a function of photon energy, while Figure 6.6 shows the mean shift (relative to event pixel center) for different split event types. Note that at low energy (E < 2 keV), both event subgroup percentage and SER shifts depend sensitively on energy. The two figures clearly show the jumps at the silicon absorption edge. Above 6 keV, the three subgroup event percentages and PIP shifts are insensitive to energy. This can be explained by the fact that, for photons with energy exceeding 6 keV, the characteristic penetration depth becomes comparable to or larger than the thickness of the ACIS BI CCD, which is only 45 μm.

The improvement in PIP determination benefits from applying the average energy-dependent shifts for different split event groups. Based on the simulations, these average shifts were calculated for different kinds of split events. Then, an offset was added to the photon impact location in chip coordinates according to charge split morphology and photon energy. This SER modification was referred as “energy-dependent” SER (EDSER).

The implementation of this EDSER approach is same as static SER, except as to how to assign the PIPs for split events. In energy dependent SER, photon energy and split event type were used to as index, to search the corresponding PIP shift, in the look up table built by CCD models. Event grade determines which direction should the “new” PIP go, relative to event pixel center, as shown in figure 6.6.

The FI simulation results (at photon energy of 1740 eV) are shown in figures 6.7, 6.8 and 6.9, to compare with BI results shown in figures 6.4, 6.5, and 6.6. Comparing the counterpart plots for BI and FI devices, one can see that split events in FI devices are significantly less, and only occurred when photon impact positions are fairly close to pixel boundaries. In addition, the branching ratio and split event shifts are more sensitive to photon energy. For BI CCDs, both subgroup event percentage and mean PIP shift depends sensitively on energy, at low energy (E < 2 keV). The 3 subgroups of split event percentages and PIP shifts are insensitive to energy for E > 6 keV. In contrast, ACIS FI CCDs are much thicker, with large depletion depth (~ 70 μm). Therefore, the branching ratios and PIP
shifts depend sensitively on energy over most of the CXO/ACIS bandwidth.

### 6.4 Charge Split Dependent SER

Figure 6.4 shows that even for the same event type, the photon landing area is widespread. By assuming the charge cloud has Gaussian shape, one might imagine that photons that land close to split boundaries could generate more charge in the split pixels. Therefore if the charge split proportion can be parameterized as a function of photon impact position, in addition to the photon energy, the SER performance could be further improved.

Simulations show that, for a split event, the proximity to the split boundary of a photon impact position is related to the proportion of the charge deposited in split pixels relative to the total charge generated by the photon. This fact provides motivation for an SER algorithm that is both energy and charge split proportion dependent. Figure 6.10 shows distances of PIPs (relative to split boundaries) as a function of the charge split proportion, for three types of split events. ACIS CCD models were used for these simulations, at a photon energy of 1740 eV. The simulated results are shown in the left and right columns, for BI and FI devices respectively. The measured fraction is the charge fraction of a split pixel relative to total charge generated by the event, including all split charges that exceed the split threshold. For 3- and 4-pixel split events, the charge fraction in both horizontal and vertical split pixels was measured independently. The charge fraction in the diagonal split pixel of the 4-pixel split events was not measured, since the fractions from the other two split pixels already provide information about photon landing locations.

Figure 6.10 shows the relationship between PIP distances (relative to split boundaries) and charge fraction in split pixels, for 2-, 3- and 4-pixel split events. Note that the horizontal and vertical split pixels are not distinguished. This means the probability of charge cross-talk to up-down or left-right neighboring pixels are assumed identical\textsuperscript{26}. From this equal-

\textsuperscript{26}Even though the pixel physical boundaries are different in the two perpendicular directions, i.e., one boundary is provided by channel stops, while the other is caused by the gate(s) with lower voltage, CCD simulations don’t show obvious split property differences for these different boundaries.
Figure 6.7: The photon landing locations for different split events, according to FI CCD simulations. Simulated phones have monochromatic energy of 1.74 keV. Note that the axes are in the unit of pixels.
Figure 6.8: The split event branching ratio for FI ACIS CCDs in terms of energy. Simulations are carried on MIT FI CCD model. Simulated photons have energy range from 0.3 to 12 keV. The attenuation length is overplotted in units of 50 microns.
Figure 6.9: FI ED SER shifts vs. energy. The mean shifts from pixel centers of the three subgroups of split events, in terms of photon energy.
probability assumption, it is assumed that functions of the distance between PIP and the split boundaries and charge split proportion are the same for both directions, for the same split-event subgroups, at the same energy.

Figure 6.10 also shows that, with only energy information, the PIP uncertainty is relatively big since it includes all "local" uncertainties. By including charge split proportion information, one can divide the uncertainty into local uncertainties, i.e., the uncertainty at each split fraction. For example, the 3-pixel split in BI devices, (the middle panel of the left column), the total uncertainty is about 0.4 pixel, while the local uncertainty at 0.4 split fraction, the uncertainty is only about 0.03 pixel. Therefore, including charge split information, the SER method will greatly reduce PIP uncertainties.

The charge split dependent SER ("CSDSER") method was developed, based on simulations using both BI and FI CCD models. Simulations were performed at each energy (as described in page 79), and derived functions of PIP proximity (to split boundaries) and charge split proportion for all three split event subgroups. The function describes PIP offset in terms of split charge fraction for a given CCD type, split-event subgroup, and photon energy. The functions are actually derived by polynomial regression at second order, and the coefficients were saved as look up table, for individual split event type at each energy step.

The implementation of this CSDSER is similar to that of energy-dependent SER, except for the "new" PIP assignment strategy. For a certain split event, the photon energy and event grade were used to locate the look up table (built by the models), and then the charge proportion in each split pixel was calculate, and used to calculate the PIP offset from the saved coefficients. Then the calculated PIP change was assigned to the correct direction according to the event grade.
Figure 6.10: The distance of photon landing locations from the split boundaries as a function of charge split proportion for three split event types. The photons have energy of 1740 eV, and simulated with MIT BI (left column) and FI (right column) CCD models. The dots in the panels represent the photon landing location (relative to split boundaries), while the red lines are the local averages of the PIPs, and the blue lines are the polynomial regression curves of the local averages.
6.5 Pixel Concept after SER Application

The Oxford dictionary defines pixel as picture element, the smallest discrete element of an image or picture. In CCD terminology, pixel is defined as a physical photosensitive cell, the smallest unit to describe the charge collection location. A CCD pixel in 2-D imaging arrays typically has rectangular shape, constrained by rows and columns.

The smallest unit specifies uncertainty — beyond that point, any value is an estimation. When one measures a table length using a ruler, for example, in which the smallest scale is millimeter. If his measurement is 12.9 mm, he knows that 0.9 mm is an estimation, and the actual length is somewhere between 12 and 13 mm. Therefore the uncertainty of this measurement is ± 0.5 mm, or 1 mm, which is the smallest unit of the ruler.

The pixel is the smallest unit in a CCD, and specifies the uncertainty of a photon landing location. In an ideal case (only one photon, no cross-talk and/or fluorescence), if charge was collected in pixel $[i, j]$, we will say that the photon was absorbed in this pixel, and can be anywhere within this pixel. In other words, the PIP possibility is uniformly distributed within the pixel. One could say the uncertainty of the photon impact position is ± $1/2p$, where $p$ is pixel physical size. Therefore, the PIP uncertainty is pixel limited, and has the same size and shape as the pixel.

After applying SER, the PIP uncertainty is actually smaller than a pixel, and conceptually means that the post-SER “pixel” is smaller than the CCD physical pixel size. In other words, SER algorithms can’t change the physical pixel size, but reduce the PIP uncertainty, thereby conceptually making the pixel size smaller.

The concept of the pixel is also related to as uncertainty distribution. Before SER application, the PIP uncertainty is uniformly distributed within the pixel. After SER, the PIP uncertainty is not uniform anymore, within its conceptual pixel. Instead, the distribution is condensed in the center, with an irregular shape that may not easily be represented by simple mathematic functions.
Figure 6.11: Differences between actual photon impact positions and processed event assumed locations for 1.74 keV events, in Chip coordinates. 1st panel (from left): ACIS assumed PIP; 2nd panel: correction using corner events only (Tsunemi et al. 2001); 3rd panel: static SER correction; 4th panel: EDSER correction; 5th panel: CDSER correction. The panels are in units of pixels. The top row panels are for BI devices, while the bottom row panels are for FI devices, for 4000 (BI) and 5000 (FI) photons with uniformly random landing positions.
Figure 6.11 shows the improvement of photon impact position accuracy, defined by differences between actual PIPs with repositioned PIPs, after applying various SER method in Chip coordinates. The calculation is based on simulated data from BI and FI CCD models, at an energy of 1740 eV. For comparison, the original ACIS assumed PIPs (always at event-pixel centers) are included. Each panel includes all three subgroup events, i.e., 13 "viable" event grades. The plot axes are in ACIS pixel units, i.e., 0.5 difference represents 12 μm, and indicates photons that interacted near the pixel boundaries. The first panel from left shows the difference of actual PIPs with unrandomized, standard-processed PIPs which are assumed to lie at the event pixel centers; one can see the expected uniform random distribution within the pixel.

The second panel is the difference after applying Tsunemi et al. (2001) model, in which only corner split events were repositioned. A big improvement for the small fraction of events that occur near corners can be seen. However, due to the small proportion of corner split events, there is no correction for most events. This fact is more obvious for the FI simulations. The third panel shows the difference after the static SER correction, in which the 2-pixel split events also were repositioned. For FI devices, SSER results in a "#"-shaped structure, because the uncertainty of 2-pixel events can only be minimized in one direction. However, the smaller PIP differences of the SSER method relative to the Tsunemi et al. (2001) method are apparent, with the improvement more obvious for BI devices.

The fourth panels (from left) of Figure 6.11 demonstrate the PIP differences after EDSER for BI and FI devices. Compared with static SER (the third panels), BI data displays a more concentrated structure in the center, indicating the split events were relocalized more accurately, and suggesting that the energy dependent SER method will improve SER performance, via better PIP determination. However, one doesn’t see the same improvement for FI data, indicating that EDSER may not yield much gain over SSER, for FI CCDs.
The right most panels in figure 6.11 show the simulated PIP uncertainties after charge split dependent SER correction for BI and FI devices. The improvement in PIP determination for this panel can be seen, especially for BI devices, compared with corrections from other SER methods. Figure 6.11 indicates the potential image quality improvement that can be achieved, by using static, EDSER and CSDSER.

How does one express the size of a non-uniform distribution? Defined by its boundaries or extremes? Clearly, no, just as one can’t say a Gaussian distribution has a size of infinity. Instead, normally the FWHM or standard deviation (σ) is used to represent its size. The same idea holds for post-SER PIP uncertainty distribution here, as the size (i.e., a conceptual pixel size) cannot be simply defined from its borders, but is related to its shape and probability distribution.

The standard deviation of a random variable can be estimated by root mean square (rms), from a large amount of given samples. Equation 6.1 defines root mean square of \( N \) samples for a certain random variable, where \( \bar{x} \) is the mean value, and \( x_i \) is the \( i^{th} \) random number of the distribution.

\[
rms = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (x_i - \bar{x})^2}
\]  

(6.1)

Root mean square defined in equation 6.1 can be used to numerically estimate pixel “size”, i.e., the uncertainty of the photon impact position. In this case, \( x \) stands for actual and estimated PIP difference. Calculations show that rms is 0.289, 0.242, 0.153, 0.137, 0.131 units, for intrinsic ACIS pixel, BI TSER, SSER, EDSER, and CSDSER conceptual pixel, respectively. Here the unit is \( \text{pixel/rms} \), i.e., a square pixel is equivalent to 0.289 rms.

Similarly, conceptual pixel size can be estimated by rms values for FI devices after various FI SER algorithms. Simulation shows that rms is 0.278, 0.226, 0.225, 0.226 units, after applying FI TSER, SSER, EDSER, and CSDSER method, respectively.

Figure 6.11 also indicates the post-SER “pixel” shape after applying various SER methods, for photons at energy of 1.74 keV. It also indicates that the post-SER pixel shape and
size are not only device type (FI or BI) and SER approach dependent, but also photon energy dependent.

6.6 Evaluation

The PSF size at each stage can be calculated from figure 4.1, by forming a 2-D image of each panel, and fitting into a Gaussian function. The PSF sizes are 0.29, 0.427, 0.625, and 0.490 for HRMA, telescope, after standard ACIS pixelization, and after SER (for BI charge split dependent method, see chapter 6.4), respectively (figure 6.12). Therefore, according to equation 8.1, the improvement can be as much as 62.1% for on-axis monochromatic sources at energy of 1.74 keV, was imaged by BI ACIS devices. However, the improvement varies in terms of source spectrum, location, employed CCD type, and SER method.
Figure 6.12: PSF scatter plot at different stages, i.e., after HRMA (UL panel), telescope (HRMA + aspect blurring; UR panel), after default ACIS pixelization (LL), and after pixelization of BI CSDSER (LR). The simulations are at ACIS-S3, for photons at the energy of 1.74 keV, and with 0''.07 aspect blurring factor.
Chapter 7

The SER performance Simulations

7.1 MARX with MIT ACIS models

MIT ACIS simulators were not designed to cascade MARX simulation. Therefore there is no direct combination between MARX output and CCD simulator input. The only way to combine the two suites of simulators is to take a detour. Thus the methods here are time-consuming.

As mentioned before, MARX suite simulates the photon collection via the telescope mirrors, aspect solution, optical block filters and detector. The output of the MARX simulation is native binary files, each of which has different attributes of the detected photons, like arrive time, grazing angle, detected energy, location, etc. Unfortunately, the output doesn't include the charge cloud size and event grade information. So MARX simulations cannot be used directly for SER analysis.

Even though the MIT CCD models provide subpixel photon landing location and charge split information, the ACIS simulators are self-independent suites which only need energy feeding, along with other CCD operating condition parameters. The models will randomly generate photon interact locations, and assume the photon beam is perpendicular to the CCD surface. Therefore there is no direct interface between MARX simulations and the CCD simulator.
In order to merge the two simulators together, the CCD model creator, Dr. Gregory Prigozhin, made great efforts to make a few crucial changes, in both input and output. The photon incident location and directions were added to input parameters, while photon incident subpixel location, signal amplitude in pixel island were added to simulation output.

Even though each ACIS CCD chip has different orientation and tilt angle relative to telescope's optical axis, the photon incident angle is very small (less than 5 degree). Adding tilt angle to incident photons results in negligible differences relative to normal incidence. Therefore the photon incident angle was set to 90 degrees, i.e., perpendicular to CCD surfaces, for all combined simulations.

Even with those changes, CCD simulators cannot take the MARX output directly. An IDL (interactive database language) program was designed to control and merge the two together. The IDL program takes the MARX outputs, including photon energy, location (in Chip coordinates), and calls the CCD simulator to simulate individual photons. The dataflow of the merged simulation is shown in figure 7.1.

The SER performance simulation includes two steps; the first step of the combined simulation is "detecting" an X-ray source through MARX simulation, in which the detector was set to "ideal"\(^{27}\). The binary files of the MARX output characterize properties of individual photon, such as energy, grazing angle, trajectory, etc. In addition, the aspect solution (telescope pointing history) was simulated by MARX.

The second step after MARX simulation is photon detection simulation. This step is actually done by an IDL program, which mainly controls ACIS simulator, and does the following functions at same time:

1. Read in required photon properties. Photon energies and landing locations in Chip coordinates are indispensable for CCD simulations. These photon attributes were saved in individual binary file by MARX.

2. CCD QE simulation. Even though CCD model has intrinsic QE assumption, the

\(^{27}\)Ideal detector has unit quantum efficiency, such that every incident photon would be detected.
Figure 7.1: The flow chart of the MARX+CCD simulation for evaluating subpixel event repositioning algorithms.

Random number generator always starts with the same random seed for each simulation. Therefore, QE is always unity in simulations when simulating one photon only. In order to simulate the CCD's QE, a random number will be generated and compared to the CCD's QE at this energy, to determine whether the photon is detected.

3. Photon simulation. Once the random number is lower than the QE value, the photon's information will pass to the CCD simulator, along with the specifications of CCD's operating condition.

4. Read in the CCD simulation results, which include detected photon energy, fit grade, PHA (Pulse Height Amplitude), and PHAS.

5. Project Chip location to other coordinate systems. Using the programs originated from MIT Center for Space Research (G. Allen, private communication), to calculate
Detector and Sky coordinates from photon location at Chip coordinates, combined with telescope pointing information provided by MARX aspect simulation.

6. Save event list file. Combining the information from MARX and CCD simulations, the event list was created for all “final” detected photons, and saved as a “fits” file such that standard CIAO tools can be used for analysis.

7.2 MARX and MIT BI CCD Model Simulation Results

In order to predict the SER improvement as a function of source off-axis angle, branching ratio, and total event counts, simulations with only one changing parameter are necessary. This is the motivation of merging the two simulators too. In addition, binary X-ray source simulations were performed to predict the power of SER methods in improving angular resolution for observation of binary star systems.

The simulation processes are time-consuming but straightforward. The purpose of the first simulation is to evaluate SER improvement tendency when source off-axis angle changes, while other parameters like split event percentage and total source counts stay constant. The simulation results are shown in figures 7.2 and 7.3. In the simulation, 50 point sources with realistic spectral distribution (see below) at positions ranging from on-axis to 160 arcseconds off-axis were simulated, in steps of 3".2. The MARX telescope “internal dither” mode was used, with standard (default) values of 1000 and 707 second dither periods in RA and DEC directions, respectively, and an 8 arcsec dither amplitude in both directions.

The telescope roll angle was set as $-4.755$ degree, and nominal RA and DEC are 170.522 and $-24.777711$ degree respectively. The source flux, 0.000080 photons/sec/cm$^2$, is same for every source; the observation time for each source is 30 kilo-seconds.

Each source has exact same spectrum too, i.e., the average spectrum from 20 sources

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28 CIAO, Chandra Interactive Analysis of Observations, is the flexible, multi-dimensional software to analyze the data that Chandra returned (http://cxc.harvard.edu/ciao/).
extracted from BI ONC observation (obsID 04). The 20 sources are from table 8.3 (Li et al. 2003), excluding sources 5 and 6, which are likely contaminated by pileup. Each source spectrum is normalized, then added together and formed the simulated spectrum, as shown in figure 7.2. The bottom panel of figure 7.2 illustrates that other parameters, like branching ratio and total source counts, stay fairly stable; and the split event percentage is in a good range that keeps SER working really optimally. This indicates that source off-axis angle is the only important parameter varying in the simulation, allowing one to test SER behavior with only source position changes.

The top panel in figure 7.3 shows how the source FWHM size changes before and after applying various SER methods. The source size, FWHM, is calculated by fitting individual source into a 2-D Gaussian function (shown in equation 8.2). Both the pre- and post-SER source size is bigger when source off-axis angle is larger, indicating that HRMA PSF size is bigger at larger off-axis angle. In addition, source size differences between pre- and post-SER, even the differences between various SER methods, are smaller when source position is further away from on-axis. These facts suggest that SER performance will be less significant at large off-axis angle. The predication is confirmed by the bottom panel, which shows the SER performance as a function of source off-axis angle. As expected, the improvement goes down quickly when off-axis angle increases, for all four SER methods, because the telescope’s PSF is broader at larger off-axis angle. However, one still can see 20% improvement for sources as far as 2.5 arcminutes away.

Figure 7.4 shows the improvement histogram for various SER methods. One can see that modified SER algorithms have significant improvement relative to the Tsunemi et al. (2001) model, and the advantage of the modified methods is already shown in figure 7.3, from both source FWHM size and improvement measurement. However, the improvement within the modified SER methods is marginal; CDSER is slightly better than EDSER, and EDSER is slightly superior to SSER. This can also been seen in table 7.1, which lists how many sources have better performance for one SER method relative to the other,
Figure 7.2: MARX+MIT BI CCD model simulation for point sources. Top: the simulated point sources spectral distribution. This spectrum represents the averaged spectral distribution from 20 sources in BI ONC observation (obsID 04). Bottom: the branching ratio and total event of the simulated sources versus off-axis angle. Note that the total event was normalized to 0.5, corresponding to 1226 detected photons. And the corner split events consist 3- and 4-pixel split events.
Figure 7.3: Results of MARX+MIT BI CCD model simulations. Top: the FWHM of the simulated sources shown in figure 7.2 versus off-axis angle, before and after applying various SER methods. Note that all FWHMs increase with off-axis angle, indicating that HRMA PSF size is a function of off-axis angle. Bottom: the improvement of various SER methods vs. source position. The decreasing tendency for improvement at large off-axis angle indicates that the aspect blurring and increasing HRMA PSF size, rather than pixelization effects, dominate CXO/ACIS PSF.
Figure 7.4: MARX+MIT BI CCD model simulations. Top: the improvement (in percentage) histogram for various SER methods. Bottom: "Box and whisker" plot for FWHM improvements using various SER methods. The symbols represent 25%, 50%, 75% percentiles of each group (boxes), as well as the mean values (circles with pluses signs), and the data range (horizontal lines).
Table 7.1: Comparison of various BI and FI SER methods.

<table>
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<th>Off-axis range</th>
<th>CCD type</th>
<th>CSD vs. ED</th>
<th>CSD vs. SSER</th>
<th>ED vs. SSER</th>
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<td>50 sources</td>
<td>0—158″.7</td>
<td>BI</td>
<td>0.996</td>
<td>68%</td>
<td>0.367</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FI</td>
<td>0.954</td>
<td>56%</td>
<td>0.954</td>
</tr>
<tr>
<td>25 sources</td>
<td>0—78″.5</td>
<td>BI</td>
<td>0.990</td>
<td>64%</td>
<td>0.059</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FI</td>
<td>0.990</td>
<td>56%</td>
<td>0.990</td>
</tr>
</tbody>
</table>

Notes. —

a) Probability that the distributions of FWHM improvement are identical under the two SER methods, as determined from a K-S test.

b) Percentage of sources for which CSDSER FWHM improvement is larger than that of EDSER.

c) As in a), for CDSER compared to SSER.

d) As in a), for EDSER compared to SSER.

for all 50 simulated sources. For comparison, the first 25 sources within 78″.5 are listed, which indicates that the modified SER methods show bigger difference at smaller off-axis angle. In addition, Kolmogorov-Smirnov (K-S) test was conducted, numerically providing information of how identical between two different SER techniques (Li et al. 2004).

Another simulation carried was to simulate the SER performance when split event percentage changes while source locations and total events stay constant. At this time, the source locations were maintained at same point, 5.2 arcsec away from optical axis, but the source spectrum is changing in order to modify the split event percentage. Other simulation parameters are same, such as observation time, source flux rate, dither pattern, etc.

As discussed in previous chapters, photon energy is related to absorption length directly, which corresponds to the branching ratio. This provides a way to control branching ratio, i.e., by changing photon energies to vary the split event percentage. Forty monochromatic point sources at different energies were simulated, with energy ranging from 0.3 to 6.0 keV.
Figure 7.5: MARX+MIT BI CCD model simulation showing split event percentage curves as the function of energy. Note that corner split events include both 3- and 4-pixel split events; split events include corner and 2-pixel split events. The attenuation length is included to show how the branching ratio is modulated by average photon absorption length.

The energy loci were not uniformly distributed in the energy range, but have more sampling where absorption length is changing rapidly. Figure 7.5 shows how the split event percentage changes as energy increases, for the forty simulated monochromatic sources. The absorption length was included to compare how the branching ratio changes as the attenuation length changes. Table 7.2 describes the simulated source information, including the branching ratio and improvement after applying charge split dependent SER.

Figure 7.5 shows how the branching ratio varies as energy changes. The plot shows that there are two significant stages of branching ratio: unstable and stable stages. When the photon energy is less than the silicon absorption edge, the split event percentage increases rapidly as energy increases, forming the unstable stages. Note that when the energy is very small (less than 0.38 keV), there are no corner split events at all. When photon energy is significantly larger than the silicon absorption length, the percentage of all kinds of split events changes slowly as photon energy varies, and forms stable stage.
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Table 7.2: Event branching ratios for the simulated 40 sources. Note that the improvement is from comparing source sizes (FWHM) before and after applying charge split dependent SER method.
Figure 7.6: MARX+MIT BI CCD model simulation illustrating SER improvement versus split event percentage. Note that the diamonds are the simulated monochromatic sources, while the red dash-dotted line is the regression curve by polynomial fit. In order to display more details in when the split percentage is about 70%, a smaller window was drawn in the lower right corner showing SER performance when split event percentage is in the range of 55 - 80%.

The reason for underlying this phenomenon is the charge cloud size. As discussed in chapter 3, charge cloud size is proportional to photon energy and diffusion time. In this case, when a photon with small energy hits a BI device, statistically the photon will be absorbed near the back surface, and generates a small charge cloud with small amount of electrons. However, the diffusion distance is fairly large, and the final charge cloud at the collection stage will be large too. Why are so few corner split events collected, then? Because the number of electrons is small, and the charge cloud is diluted. Thus, even though the cloud spreads out to neighboring pixels, it doesn’t have enough electrons to exceed the split event threshold in these pixels. From the plot we also see that the QE is relatively small at low energies, because often there are too few electrons within these charge clouds to surpass the event threshold.

Figure 7.6 shows the CDSER improvement as a function of split event percentage
Figure 7.7: MARX+MIT BI CCD model simulation illustrating SER improvement versus 2-pixel split event percentage. Labels are as in figure 7.6. A smaller window drawn in the lower right corner shows SER performance when the 2-pixel split event percentage is in the range 40 - 60%. The inner plot indicates that SER improvement is insensitive to 2-pixel split event percentage when in the range 40-60%.

(SEP) in the simulated observations. The plot shows that the improvement curve is logarithmic in form, increasing quickly at small SEP value, but slowing down at higher SEP value.

Since split events include 2-pixel split events and corner split events, similar curves are plotted in figures 7.7 and 7.8. In these figures, the SER improvement in terms of two-pixel and corner split event percentage was plotted, respectively. Figure 7.7 displays a logarithmic trend line similar to that seen in 7.6. However, figure 7.8 is quite different from the previous two. The reason is that almost no corner split events are detected among the first eight sources (i.e., the eight sources with the smallest SEP), so the improvement for these sources almost exclusively relies on two-pixel split events.

In order to investigate SER performance as a function of total source counts, an additional series of simulations was carried out, in which observation time was varied.
Figure 7.8: MARX+MIT BI CCD model simulation illustrating SER improvement versus corner (3- or 4-pixel) split event percentage. Labels are as in figure 7.6. Note that there are no or very few corner split events when the energy (or absorption length) is small. At the bottom, another window shows SER performance with improvement range limited to 20 - 70%.
Figure 7.9: Results of MARX+MIT BI CCD model simulations: SER improvement and source FWHM versus total source counts. In addition, the improvement versus observation time is also plotted (the red circle with cross inside to emphasize the equivalence of total source counts and the combination of source flux and total exposure time).

For these tests, a point source at 5''.2 away from optical axis, with flux rate 0.000080 photons/sec/cm², and spectral distribution shown in figure 7.10 (top panel) was the subject of simulated Chandra/ACIS-S3 observations for 10, 20, 100, 200, 500, and 1000 ks. Other simulation conditions, such as dither pattern, roll angle, etc. were kept the same as in the first simulations previously described. Figure 7.9 shows the FWHM improvement as a function of total source counts. As expected, SER performance is independent of total source counts, which is related to both observation time and source flux rate.

7.3 MARX + BI ACIS Model Simulations: Binary Systems

One way to demonstrate that SER repositions the photons accurately is to apply SER on binary star systems in which both stars emit X-rays. Such binary system simulations were performed by combining MARX and MIT BI ACIS CCD model. These simulations allow
one to test how SER enhances CXO’s resolving power for binary stars. A series of binary systems were simulated, with component spectra as shown in figure 7.10.

The simulations were performed as following steps:

- Simulate each component at a location and intensity (count rate).
- Combine the two individual (component) simulations into one.
- Use MIT BI ACIS model to simulate photon detection.

In all simulations, component A is the “north” component which is either fainter than or has the same intensity as component B, the “south” component. The center of component B was always fixed with off-axis angle of 1”, while A was fixed with a certain distance (north) away from B. Observations of both components were simulated with 20 kilo-seconds
exposure time, and the flux rate was adjusted so that the total number of detected photons (for both components) was around 1000 counts. Thus, in the cases of equal intensity, each component has about 500 photons detected, while for the unequal cases, the intensity ratio for components A and B is about 3 to 7, i.e., 300 photons versus 700 photons.

Figure 7.11: MARX+MIT BI CCD model simulations for the case of a binary system with equal intensity components. Component A refers to “north” star, while component B refers to “south” star. The separations between the two components is 0.3, 0.7, 1.0 arcseconds, respectively for panels (a), (b) and (c).

Figures 7.11 and 7.12 show the resulting predicted CDSER performance in distin-
Figure 7.12: Results of MARX+MIT BI CCD model simulations for the case of a binary system with unequal intensity components. Component A refers to “north” star, while component B refers to “south” star. The intensity ratio between components A and B is about 3:7. The separations between the two components are 0\textquotedblchar.3, 0\textquotedblchar.7, and 1\textquotedblchar.0, respectively for panels (a), (b) and (c).
guishing binary stars. The simulated images show that at 0''.7 separation, either equal or unequal density component can be clearly separated by SER, while the separation can be barely seen before applying SER. The separation 0''.7 corresponds to about one and a half ACIS pixels.

Figure 7.13: zeroth-order CXO/HETGS image obtained for the binary wTTS system HD 98800, before (left) and after (right) applying BI charge split dependent SER. After applying SER, the components are well resolved, despite their 0''.8 proximity and an X-ray flux ratio \( \sim 5 \). The pixel size in these images is 0''.125, and the image greyscale and contour levels are identical for each pair.

Figure 7.13 displays data (obtained in March 2003, ObsID ACISF00009) from Cycle 4 CXO/HETGS GTO observations of the hierarchical quadruple wTTS system HD 98800 (a member of the TW Hya Association; \( D = 48 \) pc). The two primary components of HD 98800 are separated by 0''.8. In preliminary analysis, after applied CSDSER to the zeroth-order HETGS image, the results confirm that applying SER methods will help to identify close-separated binary components (Kastner et al. 2004).
7.4 MARX and MIT FI CCD Model Simulation Results

The FI CCD model was modified in a manner similar to that of the BI model in order to be able to combine the FI CCD model with MARX simulations. The purpose of these simulations was to understand SER performance in application to FI CXO/ACIS observations.

For the point source simulations, the source spectrum derivation is similar to that of the BI simulation spectrum. The spectrum for the FI simulations comes from FI Chandra Orion Ultradeep Project (COUP) data, which was observed by CXO/ACIS-I, in 2003 (Getman et al. 2004). Actually the spectrum, which is shown in figure 7.14, is averaged from normalized spectra of thirty-two (32) bright sources with Gaussian shape, selected from COUP data, with off-axis angle ranging from $0''.35$ to $125''.8$ (table 8.4). Although spectra used in both BI and FI simulations come from ONC sources, the sources chosen are not necessarily the same.

The simulation procedure was very similar to that of BI simulations discussed in section 7.2. In this simulation, 50 point sources with spectral distribution (figure 7.14) normalized from 32 point sources, at positions ranging from on-axis to $160''$ off-axis angle were simulated, in steps of 3.2 arcseconds. As the default, the MARX telescope “internal dither” mode was used, with 1000 and 707 second dither periods in right ascension (RA) and declination directions, respectively, and an 8 arcsec dither amplitude in both directions. The telescope roll angle and nominal pointing direction were the same as in BI simulations. The ACIS-I array was used as the focal plane detector, and the observation time for each source is 40 kilo-seconds, thus the total detected events for each source is about 1500.

The branching ratio and total source counts for the 50 simulated sources are nearly constant, as shown in bottom panel of figure 7.14, indicating that source position (off-axis angle) is the only varying parameter. The simulation results are similar to that of the BI simulation, and are as expected: as source location is farther away from optical axis, source size increases and SER improvement decreases (shown in figure 7.15). Again it was
found that modified SER methods exhibit better improvement than Tsunemi et al. (2001) model, but the differences among the three modified approaches are marginal — CDSER is slightly better than EDSER, while EDSER is better than static SER (table 7.1; figure 7.16).

7.5 Summary

The MARX + BI simulations confirm the results shown in Li et al. (2003), in that they indicate that the modified SER algorithms have better improvement than the one proposed by Tsunemi et al. (2001). In addition, the progressively better performance of SSER, EDSER, and CDSER is apparent in BI simulations, as expected, due to better PIP determination from additional photon energy and charge split information. However, the performance of SSER, EDSER and CDSER is very comparable in the case of FI devices, even though one might expect to see the improvement (e.g., of CDSER relative to SSER) theoretically. In comparison to BI devices, the lack of improvement in imaging performance under the refined SER approaches for FI CCDs is most likely due to the following factors:

1. FI devices generate fewer split events than BI devices, especially corner split events. Therefore single pixel events dominate over the better repositioned split events.

2. For soft sources, such as those simulated here, the charge cloud size is relatively small. Therefore most split events in FI CCDs are very close to the split boundaries, not widespread as in BI devices. As a result, the positional uncertainties of two-pixel split events form a long arm cross structure after applying SER. The uncertainty in the direction parallel to the split boundary is larger and remains unchanged.

3. Because of the small charge cloud, the PIP determinations of EDSER and CDSER do not provide significant advantages over the static method, as for BI devices.

4. The slight potential improvement offered by CDSER is degraded by telescope PSF,
Figure 7.14: Source spectrum and branching ratio for 50 point sources in MARX+MIT FI CCD Model simulation. Notice that source total events are normalized to 0.5, equivalent to 1516 events.
Figure 7.15: MARX+MIT FI CCD model simulations to predict FI various SER methods performance as a function of off-axis angle. The simulated sources have identical spectrum (shown in figure 7.14), count rate and observation time. The separation between neighboring sources is 3.2 arcsec in declination direction.
Figure 7.16: Various SER methods behavior comparison from the 50 sources, simulated by MARX+MIT FI CCD model. Numerical comparison can be found in table 7.1. Panels and symbols are as in figure 7.4.
which includes contaminations from both HRMA PSF and aspect blurring.

Figures 7.3 and 7.15 show that SER algorithms are highly source location dependent, i.e., all SERs have better performance for on-axis sources, and the improvement decreases when off-axis angle increases. This is because telescope PSF size increases as source position is farther off optical axis, therefore, the influence of the event repositioning decreases.
Chapter 8

Working Regime of the SER Algorithms

The simulations in chapter 7 show that, for both BI and FI devices, SER methods perform best for on-axis sources, and their performance decreases when source off-axis angle increases. In addition, split event percentage (SEP) is another factor that controls SER behavior, whereas SER performance is independent of total event counts.

Are the simulation results consistent with real CXO observations? Is the relationship between SER improvement and its control parameters (i.e., SEP, source off-axis angle) the same for simulated and CXO observed data? This chapter will explore the behavior of various SER algorithms in real CXO observations.

It is expected that the spatial resolution improvement obtained by applying SER algorithms for CXO observations depends on the percentage of the split events, especially the corner split events. The reason is that single pixel events have no improvement on PIP determination, while 2-pixel split events have improvement in only one direction, and remain same uncertainty in the other direction; 3- or 4-pixel corner split events have the most significant improvement in both directions, as they have best PIP determination from event grade information.
Fortunately, Chandra deliberately moves its pointing direction during integration time to reduce detector non-uniformity. This dither action serendipitously produces the possibility of uniform landing positions within a pixel, even for photons from point sources. Therefore, for any given source, by employing same ACIS CCD type (BI or FI), the three classes of event grade should have similar proportions, i.e., similar branching ratios, as shown by simulations in chapter 7. In addition, SER only reduces pixelization effects, by better positioning PIPs. Therefore, SER is applicable to both compact and extended sources (Kastner et al. 2002b; Li et al. 2002; Li et al. 2003), and does not depend on the characteristics of the telescope (in particular, its PSF). Even though the tests in this chapter are based on point sources in ONC, the same results should be applicable to extended sources, such as planetary nebulae and quasar jets.

8.1 Parameters of Interest

Parameters of interest that may affect the behavior of SER algorithms can come from different aspects, such as contamination contributions from PSF, detector operating conditions, source telemetry parameters, etc. In this chapter, the parameters of interest are only limited to the source itself, and include: source off-axis position — off-axis angle; source branching ratio — split event percentage; and source flux rate — total (detected) event counts.

Point sources are easy to evaluate and are available in many CXO observations. So the algorithm evaluation is mostly based on the point sources, either by simulations or from real Chandra/ACIS observations. Source brightness, source location relative to optical axis, and the split event percentage are the parameters used to evaluate the algorithm’s performance.

8.1.1 Source Counts

Photon collection is typically assumed to be a Poisson random process, and the mean value is the product of the flux rate (photons $\cdot$ s$^{-1}$) and the integration time (seconds). The image of a point source, when degraded by an imaging system (typically, represented by
PSF), is normally approximated by Gaussian functions, which is a favorite to astronomers for its mathematical tractability for calculation and evaluation, such as size (FWHM) and intensity (peak value).

PSF is a point response function of an imaging system, mainly from optical diffraction and aberration. It can also be used as a (detection location) distribution possibility for an incoming photon. In the ideal case where the system is diffraction limited (aberration free), the PSF is the Fourier transform of the optical aperture; this transform is an Airy disk when the aperture is a circle, which is most frequently the case. Therefore, the photon detection position distribution possibility is an Airy disk function in ideal cases. However, after contamination due to optical aberrations, system PSF is not Airy disk any more. Again, for its convenient tractability, Gaussian function was most often used to approximate the PSF in practice. This approximation requires enough events to accurately represent a Gaussian shape.

Source counts reflect the X-ray source intensity, or the product of photon flux rate and exposure time. Apparently, fairly large flux rate sources can be well represented by Poisson (or Gaussian) statistics, while faint sources suffer from small number statistics. However, pileup can be an issue when the flux rate is too high. Pileup is defined here as two or more photons landing in the same or neighboring pixels within an event-detection cell during a single CCD exposure. In the case of significant pileup, the detected energy is roughly the sum of the energy of the individual photons, hence resulting in a lower event-detection rate and spectrum distorted toward higher energies (Davis 2001; Kastner 1997). Therefore, based on simple Poisson statistics, a compact or point source can cause "significant" (~10%) pileup problem when count rate is of 0.2 photons per pixel per frame (3.2 seconds) (Kastner 1997).

At the other extreme, images constructed from faint sources can't be well represented by a Gaussian function, and will likely bring significant calculation errors, because the angular resolution improvement of an SER technique is estimated by comparing the FWHM of a
point source before and after applying the algorithm.

8.1.2 Event Branching Ratio

The improvement of the spatial resolution obtained by applying SER algorithms only depends on split events, because there is no way to improve PIPs for single pixel events based on their charge distributions. The most preferred events are corner split events, as they have smallest uncertainty when reassigning PIPs in both directions.

There are many factors influence branching ratios. Other than the physical property of the CCD device itself, the CCD operating condition is an important one as it was mentioned in previous chapters. Photon energy is another factor which determines initial charge cloud size and where the photon was absorbed.

8.1.3 Off-axis Angle

The focal surface of the HRMA is a curved surface instead of a flat plane. Therefore the four abutted CCD chips in ACIS imaging array have different orientation, in order to best match the focal surface. But even with this effort, the objects with large off-axis angles are actually not at optimum focus.

In addition, the HRMA PSF itself is sensitive to off-axis angle, and is designed to have optimum image quality only within a certain off-axis angle range. The PSF is broader with an irregular wing structure when off-axis angle increases. Therefore, the reduced pixelization effect through better PIP determination will be overwhelmed by the expansive telescope PSF. In other words, the telescope PSF will dominate the angular resolution for objects far off-axis.

8.1.4 Employed CCD Type

The CCD type here refers to BI and FI devices. Because of the different physical structure (see figure 3.3) and working conditions of BI and FI CCDs, a lot characteristics like quantum
efficiency, depletion region depth, charge transfer inefficiency and readout noise are different. The reason is that photon absorption and charge spreading mechanisms differ significantly for the two types of CCDs, especially at low X-ray energies. The collection of signal charge occurs near the front surface, the same one that is illuminated by the incoming photons in the FI CCD. In such devices, a far larger fraction of photons interact close to the surface of the device where electric potentials are influenced by the grounded channel-stop layer, resulting in a very different charge splitting pattern compared to the one in the BI devices. On average, for FI devices, charge clouds are formed closer to the collecting potential wells and travel shorter distances, therefore having less time to expand. Smaller charge clouds reduce the possibility of forming split events.

A thicker dead layer covering vertical charge-splitting pixel boundaries of FI CCD is another factor contributing to reduction of the share of split events. As a result Tsunemi et al. (2001) method for FI devices suffers seriously from low detection efficiency. Because the charge cloud size is very different for FI and BI devices, even for the same energy photons, consequently the branching ratio is very different (table 8.1). Various SER methods were developed based on BI and FI devices separately, and therefore, SER evaluation will be BI and FI CCD dependent.

<table>
<thead>
<tr>
<th>Event Group</th>
<th>BI CCD</th>
<th>FI CCD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single Pixel Events</td>
<td>16.3 – 30.4%</td>
<td>71.4 – 91.6%</td>
</tr>
<tr>
<td>Corner Split Events</td>
<td>20.8 – 38.8%</td>
<td>0.7 – 8.7%</td>
</tr>
<tr>
<td>2-pixel Split Events</td>
<td>38.4 – 50.3%</td>
<td>7.7 – 20.0%</td>
</tr>
<tr>
<td>Total Spit Events</td>
<td>69.6 – 83.8%</td>
<td>8.4 – 28.6%</td>
</tr>
</tbody>
</table>

Table 8.1: The branching ratio difference between BI and FI ONC sources, calculated from 21 and 62 point-like sources in BI (ObsID 04) and FI(ObsID 18) CXO data, respectively.
8.2 Test Data: Orion Nebula Cluster

The Orion Nebula Cluster, a cluster of young stars located within the Great Nebula of Orion, was the first star-forming region to be discovered in X-ray band (see references in Feigelson et al. 2002). The ONC is a loose association of more than 5,000 mostly very young pre-main-sequence stars of a wide range of stellar mass. However, due to sensitivity, resolution and bandwidth limitations, previous X-ray missions were unable to confidently distinguish between X-ray sources. Because Chandra has the capability of delivering X-ray images with unprecedented spatial resolution, the ONC studies obtained greatly improved view, from observations offered by both ACIS imaging and spectroscopic arrays (Schulz et al. 2001; Feigelson et al. 2002).

These observations yielded detections of almost 1000 well-separated point sources, with a wide range of intensity and off-axis location. Many source images can be well approximated by a 2-D Gaussian functions. Therefore, the Orion observations are the best CXO data available to evaluate SER algorithms.

8.2.1 Range of the Parameters Represented

Heuristically, as well as predicted by simulations, the resolution improvement after applying SER algorithms on a real, broadband observation is a function of three factors: Split event percentage; Source off-axis angle; and Total source photon counts. The algorithm’s working regime was constrained by those three factors. There are numerous detectable sources in ONC data, some are as faint as 3 photon counts (in one observation) per pixel in maximum, while others are located far away from nominal optical axis.

Recall (section 5.5) that the improvement is defined as

$$\Delta = \sqrt{F_B^2 - F_A^2} / F_B$$  \hspace{1cm} (8.1)

where $\Delta$ is the relative spatial improvement before and after applying SER algorithms.

By assuming that the source is a point source, and the intensity images (cumulated photon
counts) can be well estimated by Gaussian function, the source size can be well presented by FWHM. The $F_B$ and $F_A$ are the FWHMs of fitted Gaussian function from individual sources before and after applying SER algorithms, respectively. The best-fit Gaussian function has two standard deviations in the two perpendicular directions, $\sigma_\perp$ and $\sigma_\parallel$. The FWHM of the reconstructed image $F_G$ is defined as:

$$F_G = 2 \cdot (2 \cdot \ln 2) \sqrt{\sigma_\perp^2 + \sigma_\parallel^2} \approx 2.355 \cdot \sqrt{\sigma_\perp^2 + \sigma_\parallel^2} \quad (8.2)$$

Not all real CXO sources are well-shaped; some have too few counts to construct a “good” image, while others are degraded for other reasons, such as irregular PSF structure or detector non-uniformity. Such non-Gaussian shaped sources were discarded in evaluation analysis.

As mentioned before, not all the events of a source were included to construct the image. Instead, only 13 “viable” event grades were kept, and other grades were treated as caused by unrealistic events and filtered out. On average, the fraction of rejected events is about 6 percent of total events, depending on source flux rate (pileup effect), source spectrum and employed CCD type. For the brightest source in ONC, the rejected event percentage is 25%, due to its heavy pileup, which causes distorted photon energy and unrealistic charge deposit morphology.

### 8.3 Backside-Illuminated CCD data

Two BI ONC observations were obtained in 1999, with the HETG on position. Because of the diffraction introduced by HETG, only roughly 30% of the flux goes to ACIS-S3 detector and forms zeroth order image, therefore the data are less susceptible to the effects of photon pileup in the CCDs (Schultz et al. 2001). The zeroth order gating image on S3 was used here to analyze the spatial resolution improvement of BI SER algorithms as a function of the three parameters described above.

Considering the importance of reliable statistical calculations, only sources with peak
value more than 45 photons per (intrinsic) pixel were used. 22 point-like sources (see table 8.3, sorted by pre-SER source size) were extracted according to source intensity and peak value. The sources chosen represent a range in count rate from 0.0052 to 0.2791 s⁻¹, and in off-axis angle from 2°.72 to 136°.8. A qualitative improvement of various SER methods in terms of the three parameters can be seen from figures 8.1, 8.2 and 8.3.

![Graph](image)

Figure 8.1: The spatial resolution improvement, after applying various SER methods, in terms of off-axis angle for BI ONC data. Different symbols in the plot stand for different SER methods, as indicated by the notation at upper right corner.

Figure 8.1 shows the angular resolution improvement defined in equation 8.1 in terms of off-axis angle of the point sources. The plot demonstrates the decrease of the spatial resolution improvement as the source off-axis angle increases, for all SER approaches, and predicts that significant improvement cannot be achieved for sources located far away from optical axis.

Various SER methods have different performance. In general, all three modified algorithms (SSER, EDSER, and CSDSER) have significant improvement comparing to TSER, which only repositions corner split events. In addition, among the three modified methods, CSDSER has better performance than EDSER, while EDSER performs better than SSER (see table 8.2).
Table 8.2: Comparison of various BI and FI SER methods.

<table>
<thead>
<tr>
<th></th>
<th>CCD type</th>
<th>Off-axis range</th>
<th>Degree of improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>CSD &gt; ED&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>22 sources</td>
<td>BI</td>
<td>2&quot;.72—136&quot;.8</td>
<td>54.5%</td>
</tr>
<tr>
<td></td>
<td>FI</td>
<td>6&quot;.68—156&quot;.6</td>
<td>77.3%</td>
</tr>
<tr>
<td>17 sources</td>
<td>BI</td>
<td>2&quot;.72—76&quot;.3</td>
<td>52.9%</td>
</tr>
<tr>
<td></td>
<td>FI</td>
<td>6&quot;.68—96&quot;.2</td>
<td>70.6%</td>
</tr>
</tbody>
</table>

Notes.

a). Percentage of sources for which CSDSER FWHM improvement is larger than that of EDSER.
b). Percentage of sources for which CSDSER FWHM improvement is larger than that of SSER.
c). Percentage of sources for which EDSER FWHM improvement is larger than that of SSER.

Figure 8.2 is the improvement versus split event percentage. The symbols in the plot are similar to that displayed in figure 8.1. It is difficult to see any increasing improvement tendency when split event percentage increases, for all SER methods. Therefore one might presume that SER improvement is "independent" of SEP. This seems to conflict with simulation results, where improvement increases as SEP goes up. However, one might already noticed that all the selected sources in ONC data have high split event percentage, both in corner split events (20.8 to 38.8%, mean 31.0%) and 2-pixel split events (30.5 to 50.3%, mean 44.5%). So the split event percentage ranges from 63.6% to 83.8% with the mean value 75.5%<sup>29</sup>. The simulations (chapter 7) show that SER improvement is only sensitive to SEP at lower range (less than 65%), and insensitive to SEP at higher range. Therefore, the real observational tests are consistent with the simulations.

Figure 8.3 is the improvement versus total source counts. One can see that the improvement is almost independent of source counts, i.e., the tendency of the improvement versus total event counts is quite flat for the selected sources. One can expect that, for a source without suffering from small number statistics, and without serious pileup problem,

<sup>29</sup>The reason why those sources have such high split branching ratio is that the BI devices were employed, where charge cloud size is relatively larger than in FI devices. The simulated data from a high fidelity BI CCD model (see section 6.2) verified this branching ratio.
Figure 8.2: The spatial resolution improvement in terms of split event percentage for BI SER methods applied on BI ONC data.

The spatial resolution improvement by applying SER is almost independent of the total source counts, since the potential improvement in FWHM depends only on the reliability of the repositioning of individual events. This is hypothetically true since SER “should” be independent to source intensity intuitively, as long as the source is not too faint, and can satisfy the statistical criteria. This result is consistent with the simulations too.

Figure 8.4 shows the source size changes (in FWHM) after applying various SER algorithms, and their improvement histogram. The abscissa axis in upper panel is source number, sorted with the FWHM of original point source, before applying SER but after removing randomization. It, as well as table 8.3, shows that after applying SER algorithm to these data, all SER algorithms improved the FWHM for every source (except that source
Figure 8.3: The spatial resolution improvement in terms of total source counts (in logarithm scale) for BI SER methods applied on BI ONC data.

1 has no improvement after applying the Tsunemi et al. [2001] method). Furthermore, 17 out of 22 sources have better (smaller) FWHM for energy-dependent SER than static SER, and 12 out of 22 have better behavior for CDSSER than EDSER, showing that charge-split-dependent and energy-dependent SER has better capability to improve Chandra/ACIS PSF function. For comparison, the FWHMs after applying Tsunemi et al. (2001) SER model was included. As expected, all modified SER algorithms demonstrate better improvement than this original model.

To summarize, the plots of improvement versus off-axis angle, split event percentage, and total event counts are shown in figures 8.1 - 8.3. One can see the tendency of the improvement in terms of the three factors. In general, improvement will go down quickly
Figure 8.4: FWHM and improvement comparison for various BI SER methods applied on BI ONC 22 point like sources (Table 8.3). Top: FWHM of 22 BI ONC point like sources before and after applying various SER algorithms. Bottom: The improvement histogram for various SER methods.
when off-axis angle is bigger, because larger off-axis will bring bigger optical aberration, and the PIP uncertainties were dominated by the telescope’s PSF. However, there is no clear tendency of the improvement versus split event percentage at higher SEP range and total source counts. The reason to explain the uncertain dependence of improvement on high split event percentage and total event counts might be:

1. The split event is in range of 63.6% to 83.8%, which is very high, and the SER performance doesn’t show much difference at this high range.

2. after SER correction, CXO/ACIS PSF is dominated by HRMA degradation and aspect blurring, instead of pixelization effect.

3. Improvement is in fact independent of total source counts, as long as the source is not too faint such that is well characterized by a 2-D Gaussian function.

4. also, since the sources are real source points, the three parameters are changing simultaneously. In other words, when trying to plot the tendency line of a factor, the other two are changing at same time. Therefore, the inconsistency between the observational results and theoretical expectations comes from the data, which have three independent variables at the same time. Further analysis of the data shows that the sources with high split event percentage can also have large off-axis angles, which overwhelms the potential improvement due to applying SER. Since the results from BI ONC observation are very consistent with the MARX + BI CCD simulations, we can conclude that the simulations work well, and the conclusions are reliable.

### 8.3.1 BI SER Methods Working Regime

From the simulations and ONC applications, the BI SER methods working regime can be summarized as follows:

1. A study of potential improvements to subpixel event repositioning for CXO/ACIS data has been conducted. Modified SER algorithms at three levels of improvement
<table>
<thead>
<tr>
<th>Source</th>
<th>Position (J2000.0) $^a$</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th>Improvement $^f$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\alpha$</td>
<td>$\delta$</td>
<td>SSN $^b$</td>
<td>$\theta$ $^c$</td>
<td>$R$ $^d$</td>
<td>$F_0$ $^e$</td>
<td>TSER</td>
</tr>
<tr>
<td>1</td>
<td>18.36</td>
<td>22 37.38</td>
<td>91</td>
<td>55.50</td>
<td>0.014</td>
<td>0.62</td>
<td>...</td>
</tr>
<tr>
<td>2</td>
<td>15.63</td>
<td>22 56.44</td>
<td>55</td>
<td>28.48</td>
<td>0.023</td>
<td>0.62</td>
<td>38.86</td>
</tr>
<tr>
<td>3</td>
<td>17.00</td>
<td>22 32.95</td>
<td>76</td>
<td>51.15</td>
<td>0.005</td>
<td>0.63</td>
<td>37.46</td>
</tr>
<tr>
<td>4</td>
<td>15.26</td>
<td>22 56.83</td>
<td>48</td>
<td>30.30</td>
<td>0.012</td>
<td>0.64</td>
<td>42.01</td>
</tr>
<tr>
<td>5</td>
<td>16.46</td>
<td>22 22.89</td>
<td>C</td>
<td>2.72</td>
<td>0.279</td>
<td>0.64</td>
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</tr>
<tr>
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<td>23 09.86</td>
<td>E</td>
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<td>0.67</td>
<td>47.78</td>
</tr>
<tr>
<td>7</td>
<td>14.32</td>
<td>23 08.31</td>
<td>24</td>
<td>32.67</td>
<td>0.008</td>
<td>0.67</td>
<td>31.72</td>
</tr>
<tr>
<td>8</td>
<td>12.29</td>
<td>23 48.06</td>
<td>7</td>
<td>64.74</td>
<td>0.009</td>
<td>0.67</td>
<td>30.25</td>
</tr>
<tr>
<td>9</td>
<td>17.94</td>
<td>23 45.42</td>
<td>85</td>
<td>45.10</td>
<td>0.092</td>
<td>0.68</td>
<td>35.27</td>
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<tr>
<td>10</td>
<td>15.82</td>
<td>23 14.19</td>
<td>A</td>
<td>11.27</td>
<td>0.023</td>
<td>0.69</td>
<td>38.52</td>
</tr>
<tr>
<td>11</td>
<td>21.03</td>
<td>23 48.00</td>
<td>108</td>
<td>76.27</td>
<td>0.035</td>
<td>0.70</td>
<td>7.34</td>
</tr>
<tr>
<td>12</td>
<td>14.55</td>
<td>23 16.01</td>
<td>30</td>
<td>26.80</td>
<td>0.009</td>
<td>0.70</td>
<td>47.19</td>
</tr>
<tr>
<td>13</td>
<td>17.06</td>
<td>23 34.09</td>
<td>78</td>
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<td>0.71</td>
<td>28.46</td>
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<tr>
<td>14</td>
<td>15.34</td>
<td>22 15.47</td>
<td>50</td>
<td>69.09</td>
<td>0.012</td>
<td>0.72</td>
<td>22.37</td>
</tr>
<tr>
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<td>19.20</td>
<td>22 50.63</td>
<td>97</td>
<td>54.57</td>
<td>0.024</td>
<td>0.72</td>
<td>40.20</td>
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<tr>
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<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>32.36</td>
</tr>
<tr>
<td>17</td>
<td>14.91</td>
<td>22 39.14</td>
<td>40</td>
<td>48.54</td>
<td>0.007</td>
<td>0.76</td>
<td>33.43</td>
</tr>
<tr>
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<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>35.98</td>
</tr>
<tr>
<td>19</td>
<td>15.97</td>
<td>23 49.70</td>
<td>60</td>
<td>27.22</td>
<td>0.014</td>
<td>0.79</td>
<td>46.07</td>
</tr>
<tr>
<td>20</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>115.42</td>
<td>0.012</td>
<td>0.90</td>
<td>35.24</td>
</tr>
<tr>
<td>21</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>136.75</td>
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<td>20.59</td>
</tr>
<tr>
<td>22</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>120.50</td>
<td>0.009</td>
<td>1.12</td>
<td>3.66</td>
</tr>
</tbody>
</table>

Notes.—

a. Right ascension for all sources is at 5h35m; values in table are in units of seconds; Declination for all sources is at -5°; values in table are in units of arcminutes and arcseconds.

b. SSN stands for Schulz et al. (2001) source number.

c. $\theta$ = off-axis angle in arcsecond.

d. $R$ = source count rate in counts/sec.

e. $F_0$ is source FWHM (in arcsec) after removing randomization but before applying SER.

f. Various SER improvement in FWHM; here ED stands for ED$^a$SER, and CSD stands for CSD$^a$SER.

Table 8.3: Information for the sources appearing in figure 8.4.
were formulated: (1) inclusion of single-pixel events and two-pixel split events ("static" SER); (2) accounting for the mean energy dependence of differences between apparent and actual photon impact positions, based on the results of BI CCD simulations ("energy-dependent" SER). (3) dependence of the actual PIPs according to the split charge proportion in the split pixels, event type, and event energy, based on CCD model simulation results ("charge split dependent" SER).

2. All modified SER methods — static, energy-dependent, and charge split dependent SER — produce improvements in spatial resolution over those possible using an earlier static SER algorithm employing only corner-split events (Tsunemi et al. 2001). The potential improvement in image FWHM is ~50% using either of the "modified SER" algorithms described here, with charge split dependent SER and energy-dependent SER producing a marginally superior result. The relatively small improvement observed for either energy-dependent SERs, relative to static SER, suggests that under either method, the telescope blurring (including HRMA PSF and aspect blurring) — rather than ACIS pixelization — dominates image FWHM.

3. Various SER methods have similar performance tendency, in terms of source off-axis angle, split event percentage, and source total event counts. In general, SER improvement goes down when source off-axis angle increases; improvement is relatively independent of source split event percentage when SEP is in higher range, but the relationship is more obvious when SEP is at lower value. At that range, SER improvement increases when SEP increases. The degree of improvement is independent of source intensity.

4. SER techniques only take into account the properties of photon charge-splitting within CCD pixels, and do not depend on the characteristics of the celestial source (in particular, its surface brightness distribution). Therefore, SER is applicable to both compact and extended sources (Kastner et al. 2002b, Li et al. 2002). However, deconvolution
methods have been developed in recent decades for optical and IR astronomical imaging, to correct for the blurring due to telescope PSF. Burrows et al. (2000) used one technique, Maximum Likelihood, to deconvolve the ACIS-S image of SN 1987A. At present, multiscale deconvolution methods are being explored, which are more suitable to process Poisson-distributed data, and therefore may be better applicable to X-ray imaging (Willett et al. 2002; Esch et al. 2002). By combining SER techniques and such multiscale deconvolution methods, one can expect the best possible spatial resolution from Chandra/ACIS imaging.

8.4 Frontside-Illuminated CCD data

CXO has two FI observations of ONC before 2001, one was collected in October 1999 (obsID 18), another in April 2000 (obsID 1522). Those observation data are publicly available at Chandra archive. The FI ONC data were collected by ACIS-I devices, which covers larger area than ACIS-S. Because of the longer integration time, and no grating facilities involved during observation, the sources in those data have more photon counts than that in BI data, therefore have better statistical precision.

In this section, only data from observation 18 were used, because of its longer observation time (than obs. 1522). This dataset was used as a representative to evaluate SER techniques for FI data.

Figure 8.5 shows the angular resolution improvement defined in equation 8.1 in terms of off-axis angles of the point sources. Similar to figure 8.1, the plot displays decreasing tendency of the spatial resolution improvement when the source off-axis angle increases, and indicates that at far off-axis angle, the telescope PSF errors are dominated, and impede the improvement of SER techniques.

The top panel in figure 8.6 is the SER improvement in terms of the split event percentage for FI ONC point sources. The increasing tendency of SER improvement is obvious when split event percentage increases, opposite to figure 8.2, the BI counterpart plot. The
Figure 8.5: The spatial resolution improvement versus source off-axis angle for FI data. Different symbols stand for different SER techniques, as indicated by the plot notations at UR corner. Note that some points are “missed” for a certain SER method, indicating that there is no improvement at those sources by applying the specific SER algorithm.

reason is that FI data has relatively smaller split event percentage, for example, ranges from 12.5 to 26.1% for 22 FI sources. At this lower band, SER performance is very sensitive to split event percentage variation, as predicted by MARX + BI ACIS simulations.

The bottom panel in figure 8.6 shows the spatial resolution improvement in terms of source total counts. Similar to figure 8.3, the BI counterpart plot, there is no obvious tendency, and indicates that SER improvement is independent of source counts.

The spatial resolution improvement by applying SER techniques are shown in figures 8.5 and 8.6, in terms of off-axis angle, split event percentage, total source counts for front illuminated CXO data. One may also notice the similarity of the tendencies for BI and FI
observations, despite the improvement amplitude discrepancies.

Figure 8.7 and table 8.2 illustrate the performance differences among various FI SER methods, from the FWHM size and improvement difference after applying SER correction. The results show that, all three modified FI SER (SSER, EDSER, and CSDSER) methods have superior performance relative to the Tsunemi et al. (2001) model, which only corrects corner split events statically. In addition, energy dependent method has marginal advantages over the static method, while charge split dependent SER has slightly better performance than energy dependent SER.
Figure 8.6: The spatial resolution improvement in terms of split event percentage (top) and total event counts (bottom) for FI data.
Figure 8.7: Source FWHM change (top) and SER improvement histogram (bottom) comparison for various FI SER algorithms applied on FI ONC point sources.
8.5 SER Performance Evaluation Conclusions

Various SER methods have been applied on real Chandra/ACIS observations to evaluate their performance. The improvement was plotted in terms of three parameters, i.e., source off-axis angle, split event percentage, and total source counts. The off-axis angles of the displayed sources are in the range of 0 to 137" for BI data, and 0 to 157" for FI data. From figure 8.1 to 8.7, one can see that the angular resolution of the plotted sources benefit from applying SER techniques, for both BI and FI data. In addition, BI SER methods have much better performance than FI SERs, due to the higher split event percentage for BI devices. Off-axis angle significantly affects the degree of improvement, and (possibly) the split event percentage. Total source counts has no influence on the degree of improvement.

According to the improvement definition (equations 8.1 and 8.2), the degree of improvement (for modified SER methods) is about 60% for on-axis sources, and 30% for 150" off-axis sources for BI data. For FI data, it is 35% and 25% for on-axis and 150" off-axis sources, respectively (figure 8.17).

8.6 SER Applications

8.6.1 SER Application to Binary X-ray Sources

The most intuitive way to subjectively evaluate SER performance is applying SER techniques on binary X-ray sources. If the source indeed is a binary X-ray source system, the separation of the components should be more obvious after applying SER algorithms.

The binary wTTS system HD 98800 is shown in figure 7.13, before and after applying BI CSDSER method. The separation between the two components is \( \sim 0''.8 \). The same zeroth-order CXO/HETGS X-ray image is shown again in figure 8.8 (top panels), as well as the IR counterpart (bottom panels). Pre-SER and post-SER X-ray images are compared in top panels (Kastner et al. 2004). The image intensity and its contours clearly indicate that the post-SER image allows a more confident assertion that the system consists of two point
like sources. The mid-IR Keck images at different wavelength (7.9 and 10.3 µm for left and right panel, respectively) clearly show that the object is indeed a binary system. Thus, the comparison of pre- versus post-SER X-ray images with each other, and with optical/IR images, confirms that SER techniques can help to identify binary X-ray systems.

Figure 8.8: Top: Chandra/HETGS zeroth-order X-ray images of HD 98800, before (left) and after (right) SER application. In each X-ray image, pixel scale is 0\textquoteright.125, and contour levels are 0.05, 0.1, 0.2, 0.4, and 0.7 of the peak. Bottom: Keck Telescope mid-IR images of HD 98800 (Prato et al. 2001). Note that the component that is stronger in X-ray images is weaker in IR images.

Another example of an X-ray binary is the recently observed X-ray young star system Hen3-600. The zeroth-order image is shown in Figure 8.9; the separation between the two
components is \( \sim 1''.52 \). After applying CSDSER, the post-SER image clearly shows that there is much less flux "between" the two components and both appear more point like. The "bridge" remaining between the components may be due to aliasing caused by removal of photon position randomization.

![Figure 8.9: Chandra/HETGS zeroth-order X-ray images of Hen3-600, before (left) and after (right) SER application. Pixel scale is 0''.125. In each X-ray image, contour levels are 0.05, 0.1, 0.2, 0.4, and 0.7 of the peak.](image)

8.6.2 SER Application to Extended Sources

As mentioned in section 8.3.1, SER algorithms don’t depend on telescope PSF or X-ray source characteristics (other than, perhaps, split even percentage and source off-axis location). Instead, they only take into account the properties of charge deposit information within CCD pixels, for individual photons. Therefore, SER techniques are applicable to both compact and extended X-ray sources.

The static SER method has been applied to X-ray imagery of several extended young planetary nebulae (BD + 30°3639, NGC 7027, and NGC 6543, Kastner et al. 2002b; Mz3,
Kastner et al. 2003), as well as the jet in quasar 3C 273 (Li et al. 2002). All applications demonstrate improved angular resolution, and confirmed the assertion that SER is applicable to extended sources too.

NGC 6543 (Chu et al. 2001) was observed by CXO/ACIS-S3, and was chosen as a representative to test various BI SER methods. In addition, original level 1 data and unrandomized data were included, for comparison purposes.

Figure 8.10: Planetary nebula NGC6543 before and after applying various BI SER methods. Note that logarithm scale is applied, after image convolved with CXO PSF. Plotted pixel scale is $0''.25$, i.e., half size of intrinsic ACIS pixel size.

Figure 8.10 is a 6-panel plot for planetary nebula NGC6543, before and after applying various SER algorithms. The top panels from left to right are images constructed from original (standard) ACIS processed level 1 event file, event file after removing randomization, and event file after applying Tsunemi et al. (2001) SER method. The bottom panels from
left to right are images constructed from event files after applying static, energy-dependent, and charge split dependent SER methods, respectively. All images are convolved with CXO PSF, and pixel size is half intrinsic ACIS pixel size, i.e., 0.25''. All panels are presented in a log scale, at the same maximum intensity, with a color bar representing the gray-scale mapping to log intensity. The plot indicates that all three modified techniques displayed in bottom row perform well, with CDSER marginally superior.

8.7 COUP Data Analysis

The Chandra Orion Ultradeep Project combines six consecutive observations of the Orion Nebula Cluster taken in January 2003 with the Advanced CCD Imaging Spectrometer on board the Chandra X-ray Observatory. The total exposure time was 0.84 Ms and over 1600 sources are detected.

COUP data reduction started with the Level 1 event files provided by the Chandra X-ray Center. Only events on the four CCDs of the ACIS-I array were considered. Event energies and grades were corrected for charge transfer inefficiency (CTI) using the procedures developed by Townsley et al. (2002b). The data were cleaned to remove a variety of potential problem events with the grade, status, and good-time intervals filters as described in the Appendix of Townsley et al. (2003). The data are then searched for hot columns or hot pixels that are not removed by the standard processing (e.g., events below 700 eV are removed from column 3 of CCD 10), and a very coarse energy filter (eliminating events with E > 10.5 keV) is applied to remove background events (Getman et al. 2004).

Because the COUP data were obtained in a sequence of six separate "exposures", event positions were adjusted slightly in three ways. First, individual corrections to the absolute astrometry of each of the six COUP exposures was applied based on several hundred matches between a preliminary catalog of Chandra sources and near-infrared sources in a forthcoming catalog from the ESO Very Large Telescope. Second, the sub-arcsecond broadening of the PSF produced by the Chandra X-ray Center’s pipeline randomization of positions was
removed. Third, the tangent planes of five COUP exposures were re-projected to match the tangent plane of the first observation (ObsID 4395). The six exposures were then merged into the single data event file used in the further analysis. These position corrections do not affect the results of SER, as demonstrated by the comparison between FWHM for simulated and real datasets (Figures 7.16, 8.11).

There are more than 1600 separated sources in the resulting COUP observation, providing tremendous flexibility for SER method evaluations. With criteria of very good Gaussian shape, and 2-pixel split event percentage larger than 15%, 32 sources are extracted and their spectra were normalized to form the simulation spectrum (see section 7.4). Those sources are listed in table 8.4. Various FI SER techniques were also applied to COUP data after it is cleaned, CTI corrected, and merged multiple observations and the results from the 32 sources are shown in figure 8.11 and table 8.4.

On the other hand, there are many more qualified sources that can be extracted from COUP and used for FI SER evaluation. One hundred well shaped point like sources (including above 32) are used to test the SER performance. The results are shown in figures 8.13, 8.14, and 8.15.
Figure 8.11: Comparison of image FWHM size and their improvements using Tsunemi et al. (2001) model, static, energy-dependent SERs, ED and CSD SER on selected FI CXO COUP sources.
Table 8.4: Information for the sources appearing in figure 8.11.

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<th>Rd</th>
<th>F0e</th>
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</table>

Notes.— a. Right ascension for all sources is at 5°35'; values in table are in units of seconds; declination for all sources is at -5°; values in table are in units of arcminutes and arcseconds.

b. CSN stands for COUP data catalog source number (Getman et al. 2004).

c. θ = off-axis angle in arcseconds.

d. Rd = source count rate in counts/sec.

e. F0 is source FWHM (in arcsec) after removing randomization but before applying SER.

f. Various SER improvement (Δ) in FWHM; here ED stands for EDSSER, and CSD stands for CSDSER.
Figure 8.12: Improvement varies in terms of split event percentage and total event counts for COUP data after applying various SER algorithms.
Figure 8.13: The SER performance on 100 COUP sources: improvement versus off-axis angle.
Figure 8.14: FWHM changes and improvement histograms for COUP data after applying various SER algorithms.
Figure 8.15: “Box and Whisker” plot for FWHM improvement of 100 COUP sources after applying various SER algorithms. The symbols represent 25%, 50%, 75% percentiles of each group (boxes), as well as the mean values (circles with pluses signs), and the data range (horizontal lines).
8.8 Results and Comparison

In this chapter, I have calculated the FWHM of 22 bright point-like sources in BI ONC data, obtained by Chandra using ACIS-S3 for various SER methods. The sources were selected to represent a range in off-axis angle from 2".72 to 136".8, and in count rate from 0.0052 to 0.2791 s\(^{-1}\). The top panel in Figure 8.16 shows that after applying SER technique to these data, all SER algorithms improved the FWHM for every source (except that source 1, which displays evidence for pileup, has no improvement after applying the Tsunemi et al. [2001] method). The bottom panel displays 32 point-like sources chosen from Chandra/ACIS-I COUP observation, with count rate ranging from 0.0027 to 0.0799 s\(^{-1}\) and off-axis angle from 0".35 to 125".8. Results for FWHM and improvement percentage for these 32 sources are listed in table 8.4. Both abscissa axes in figure 8.16 are source number, sorted with the FWHM of original point sources, before applying SER but after removing randomization. Furthermore, COUP data process includes CTI correction (Townsley et al. 2002b), to reduce charge transfer problem in ACIS-I CCDs and to recover event grade information.

The source size, represented by FWHM, was apparently smaller after applying SER approaches on BI devices, from TSER to SSER, EDSER, and, finally, to CSDSER (Figures 8.16 and 8.17, top panels), demonstrating the capability to improve the spatial resolution of BI Chandra/ACIS imaging. The degree of improvement observed agrees very well with the predictions of the simulations. At the same time, FI devices illustrate more modest improvements, after application of SER techniques (Figures 8.16 and 8.17, bottom panels). The improved performance of static SER over TSER is evident, but from SSER to EDSER and CSDSER, the improvement is less clear. However, a small improvements in effective FI Chandra/ACIS PSF still can be seen after application of SER techniques.

Using the definition of improvement given by equation 8.1, one can quantitatively evaluate the performance of different SER methods on ONC data. The top and bottom part of Figure 8.17 shows this metric of the improvement for all SER algorithms for BI and FI
Figure 8.16: FWHM of BI (top panel) and FI (bottom panel) ONC point like sources before and after applying various SER algorithms described in this paper.
Figure 8.17: Comparison of image FWHM improvements using Tsunemi et al. (2001) model (TSER), static SER (SSER), energy-dependent SER (EDSER), and charge-split-dependent SER (CSDSER) on BI (top panel, 22 sources listed in table 8.3) and FI (bottom panel, 32 sources tabulated in table 8.4) CXO ONC data.

Chandra/ACIS sources, respectively. As expected from MARX simulations, BI data shows superior improvement for CSDSER and EDSER, while FI data only shows improvement for modified SERs, and there is no favorite among the three modified methods. Improvement for most sources in FWHM range is from 40% to 70%, and from 20% to 50%, for BI and FI CCDs, respectively, with the improvement statistically dependent on off-axis angle.
Chapter 9

Conclusions and Recommendations

9.1 Summary and Conclusions

The blurring of CXO/ACIS imaging effectively serves as a low pass filter and limits the system’s angular spatial resolution. There are three major image degradation sources contained in the point spread function of CXO/ACIS imaging:

**Mirror PSF** The blurring is caused by optical diffraction limit and optical aberrations from High Resolution Mirror Assembly.

**Aspect blurring** The blurring is caused by CXO’s intentional dither motion and reconstruction uncertainty. The convolution of the aspect blurring and the mirror PSF forms the telescope PSF.

**CCD pixelization** ACIS devices have finite pixel size equivalent to 0".492, insufficient to fully sample telescope PSF.

Because the three blurring factors are statistically independent, the system PSF is a convolution of these three sources. However, the CXO/ACIS PSF is CCD pixel size limited. In addition, the system PSF is a function of photon energy, X-ray source location (off-axis angle). High fidelity simulation tools show that for an on-axis monochromatic source at an
energy of 1.74 keV, the mirror PSF is about 0.292 (FWHM); the aspect blurring is about 0.165 (FWHM). Therefore, the telescope PSF is about 0.427. The cascaded system PSF is therefore about 0.625, which is the convolution of the telescope PSF and the ACIS pixel.

Subpixel event repositioning techniques intend to minimize pixelization effect, thus improve system's resolving power. Simulations from MARX and ACIS simulators show that, for on-axis monochromatic point source at the energy of 1.74 keV, when imaged by BI CCD, the recorded source size (FWHM) is 0.625 without SER, and 0.490 after applying BI charge-split-dependent SER (section 6.4). Therefore the resolution improvement (equation 8.1) is 62.1%, and the CSDSER method recovers essentially all of the resolution loss due to CCD pixelization.

When applying on actual observations, the performance of various SER techniques agrees very well with the predictions of simulations. In addition, the application of SER algorithms is not limited to point sources, these techniques also can be used on X-ray binary systems, and extended X-ray sources, to improve angular resolution, and therefore image quality.

In this dissertation the following contributions have been made:

- The possibility and necessity of subpixel event repositioning algorithms have been theoretically analyzed. The resolution improvement was numerically predicted via simulations.
- Tsunemi et al. (2001) SER model was modified by adding 2-pixel split events and single-pixel events, thus improved the efficiency, and SER performance as well (Static SER).
- Energy-dependent SER method was developed based on high fidelity ACIS CCD models. This algorithm utilizes photon energies, as well as event grades, to further minimize photon impact position prediction uncertainty.
- Charge-split-dependent SER model was developed based on ACIS CCD simulators.
This method utilizes charge split fractions in the split pixel(s), photon energies and event grades. This method has superior performance relative to any other SER algorithm.

- SER techniques are differentiated for FI and BI CCDs, based on the fact that FI and BI CCDs exhibit different performance.

- MARX and high fidelity ACIS models were first combined successfully to predict full CXO/ACIS imaging functionalities, providing necessary information for subpixel event repositioning.

- The performance of various SER techniques were tested on actual observations of real targets (Orion nebulae cluster, X-ray binary sources, extended X-ray sources), and simulated via MARX and ACIS CCD model simulations. The improvement in image quality measured for actual FI and BI CCD observations agrees very well with the prediction of simulations.

9.2 Recommendations

9.2.1 Making SER a Part of CIAO

Currently, SER techniques are under development and testing; and the package is written in IDL (Interactive Data Language), without supported public access. SER algorithms have been successfully applied to improve angular resolution for various Chandra/ACIS observations, such as the Orion nebula cluster (Li et al. 2003; Li et al. 2004), young planetary nebulae (Kastner et al. 2002b, 2003), and the remnant of SN 1987A (Park et al. 2002). In addition, recently developed energy and/or charge split dependent SER algorithms hold promise to further improve CXO spatial resolution. Therefore, it is necessary to make SER

\[\text{It hasbeen available at http://cxc.harvard.edu/cont-soft/software/SER(subpixelEventRepositioning).2.0.html, without thorough tests.}\]
algorithms available in a fully supported standard package, preferably as a built-in tool for Chandra Interactive Analysis of Observations (CIAO).

9.2.2 Applications to Gratings Spectroscopy

CXO has high- and low-energy transmission grating instruments (HETG or LETG), to provide high resolution spectroscopy. The grating data allows one to probe the physical parameters of emitting regions of a variety of classes of X-ray sources, to deduce source properties like temperatures, plasma velocities, structures, and even the temporal evolution of various classes of sources.

Photon energies/wavelengths are assigned based upon the diffraction angle of the events, that is, the spatial position of the events relative to the zeroth-order image (CPOG). The spectrum is created by projection of events along the dispersion axis and binning the events into wavelength bins, with wavelength determination from the standard grating equation. The spectral order can be sufficiently sorted using intrinsic energy resolution of ACIS; thus the photon wavelength can be uniquely determined when HETG or LETG are used in conjunction with ACIS (HETGS or LETGS).

The resolving power of either gratings spectrometer, as represented by the grating plus ACIS line response function (LRF), is determined by three main contributing components: the telescope PSF, effects along the dispersion direction and effects in the cross-dispersion direction of the HETG or LETG. Among them, the telescope PSF likely dominates over many wavelength ranges (CPOG), and this contribution can be further decoupled into three parts: HRMA PSF, aspect blurring, and pixelization effects. By reducing pixelization effects, SER techniques greatly improve spatial resolution for imaging, especially for BI CCDs. Similarly, by increasing photon impact position accuracy, SER techniques should improve the spectral resolution for gratings.

Preliminary results of applying SER on gratings data can be seen in figure 9.1 (courtesy of D.P. Huenemoerder). The energy-dependent BI SER was applied to the detector
coordinates of TV Crt (CXO obsID 3728) and AR Lac (CXO obsID 9), then the histogram in cross-dispersion direction was plotted. At low energy, the peak in the SER (black) histogram rises above the peak in the unrandomized data (grey) histogram at the center of the cross-dispersion counts distribution, and the wings are slightly suppressed in the SER data relative to just unrandomized. The fact that the peak of the SER histograms of spectral lines is either above or equal to the pre-SER at all energy ranges also indicates that SER is improving the pixelization, therefore the line spread function, on average.

The line profiles in AR Lac, a single point source with many more counts relative to HD 98800, are already resolved by HETGS. But line profiles are apparently unresolved in the young binary HD 98800. After applying SER to the HD 98800 spectrum, one can test whether its lines remain unresolved in velocity.

Clearly, good models of the PSF and LRF are very important for improvement evaluation. Part of further research effort will involve improving the characterization and parameterization of the PSF and LRF, in collaboration with Chandra X-ray Center research staff.
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