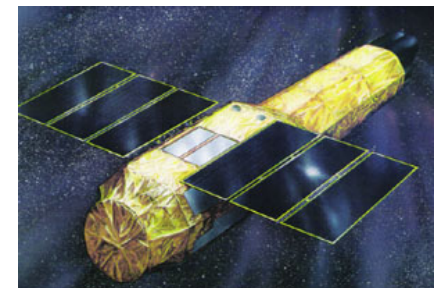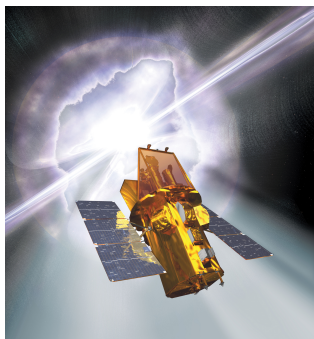# CCDs for X-ray Astronomy

Catherine Grant, MIT

5th X-ray Astronomy School

7 August 2007

OVERVIEW

- Charge-Coupled Devices: Basic Principles and Operation

- CCD Performance: Energy Resolution, Quantum Efficiency

- CCDs onboard Chandra and XMM-Newton

- Detector "Features": Pileup, Charge Transfer Inefficiency, Contamination, Background

- CCDs in Future X-ray Astronomy Missions

CCDs: Basic Principles

- CCD = Charge-coupled device
  - An array of linked ("coupled") capacitors
  - Photons interact in a semiconductor substrate and are converted into electrons
  - An applied electric field collects and stores the electrons in pixels
  - Pixels are "coupled" and can transfer their stored charge to neighboring pixels
 - Stored charge is transferred to a output amplifier and read out

Reminder: What is a Semiconductor?
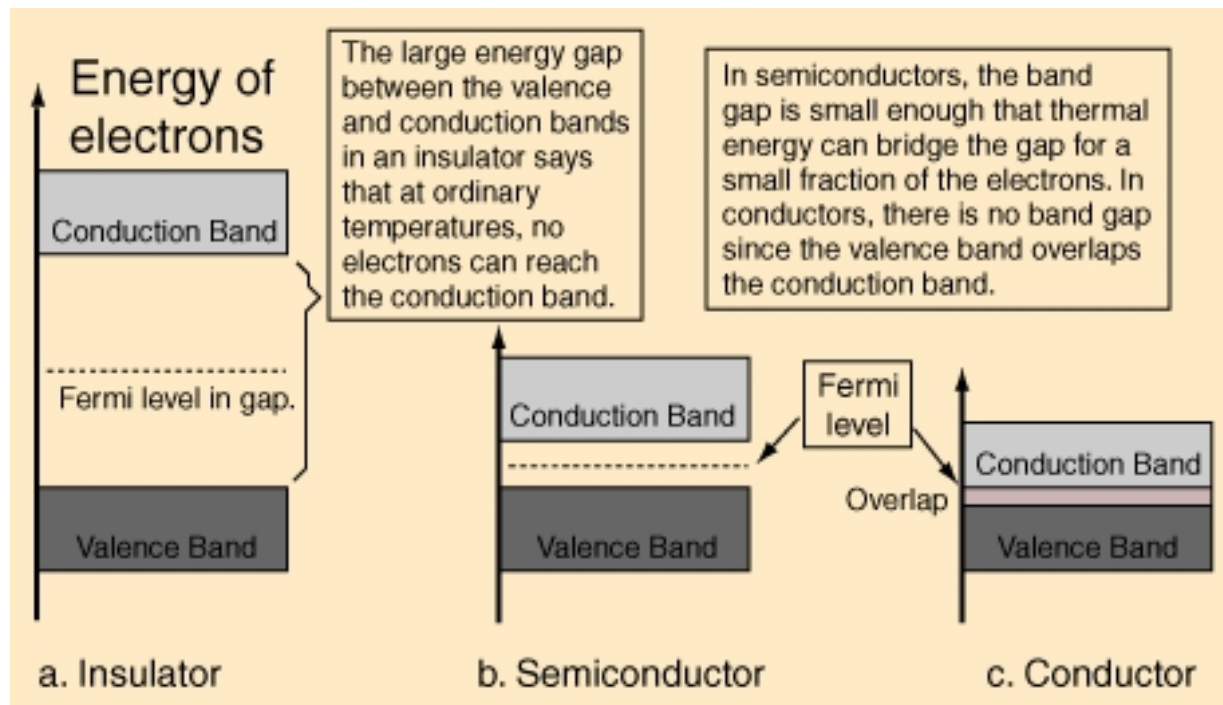
- Intermediate conductivity between insulators and conductors
- Small energy input can promote e⁻ to conduction band
- Silicon band gap ~ 1.1 eV

(From http://hyperphysics.phy-astr.gsu.edu/hbase/hframe.html   Very cool and highly recommended!)

Photoelectric Absorption in Silicon
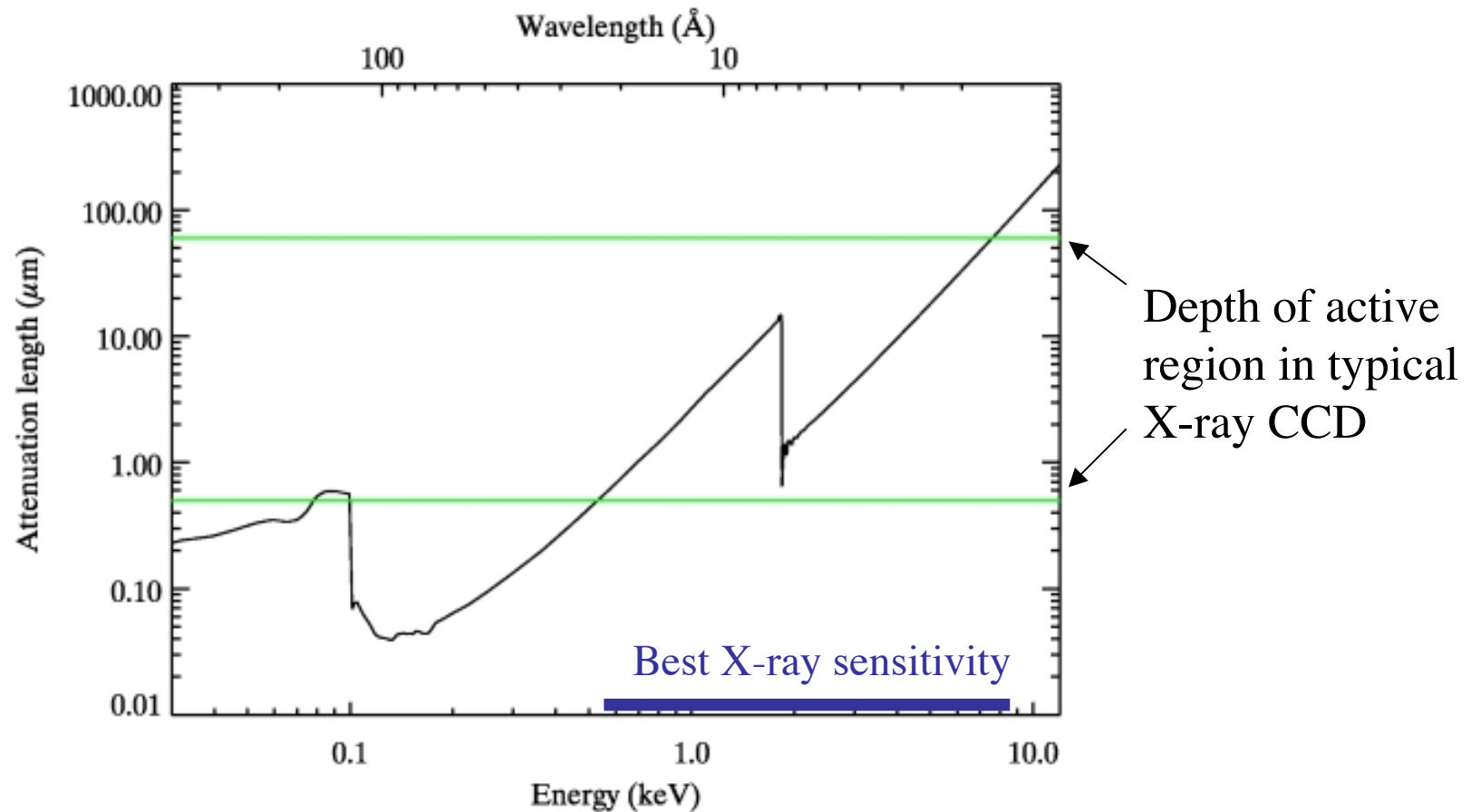
Photoelectric Absorption

- Photoelectric interaction of X-ray with Si atoms generates electron-hole pairs.
- On average: $N_e = E_x/w$
  - N_e = number of electrons
  - E_x = energy of X-ray photon
  - $w \sim 3.7$ eV/e$^-$ (temperature dependent)
- X-ray creates a charge cloud which can diffuse and/or move under influence of an electric field

A little more on Semiconductors

- Doping: add small number of impurities - increases conductivity
- n-type, excess e⁻
  - (P, As)
- p-type, excess holes
  - (B, Al)
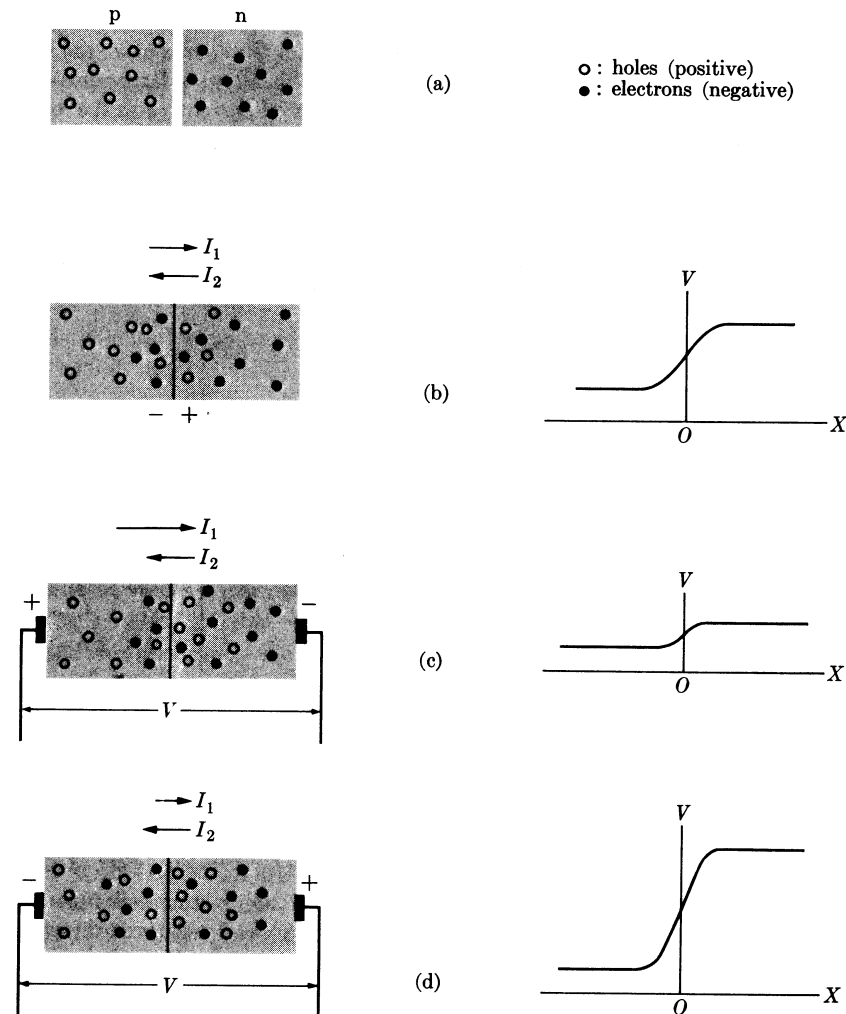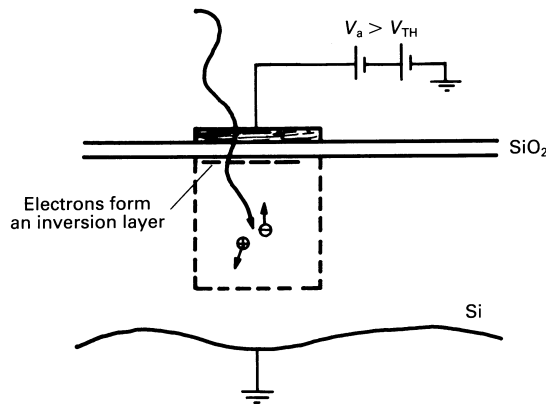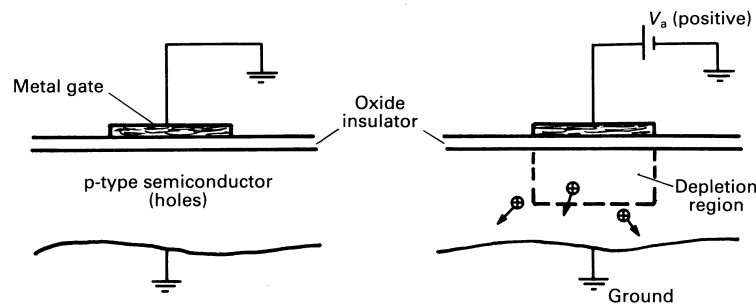- p-n junction
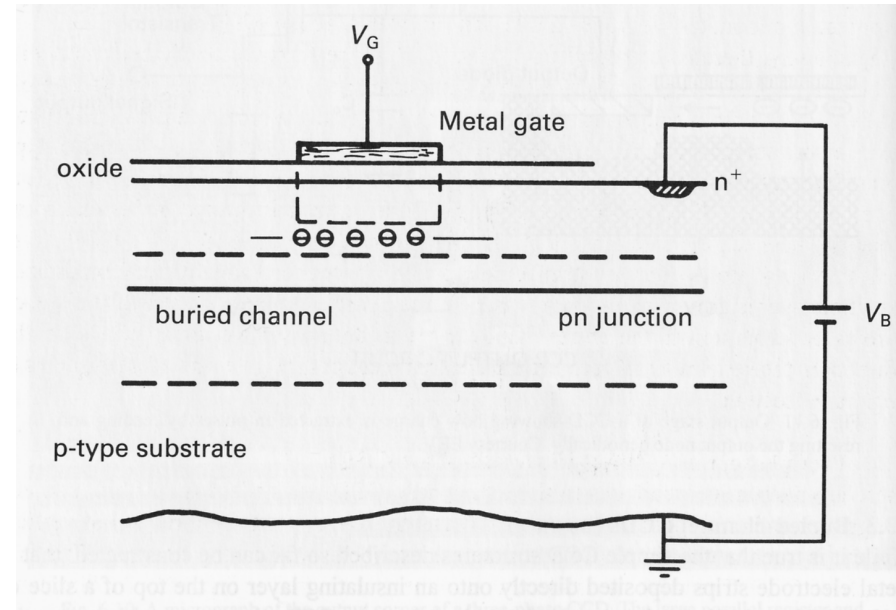 - Current depends on voltage polarity

Fig. 6-41. The p-n junction.

Charge Collection

V_a (positive)

Metal gate

Oxide insulator

p-type semiconductor (holes)

Depletion region

Ground

$V_a > V_{TH}$

SiO_2

Electrons form an inversion layer

Si

A single metal-oxide-semiconductor (MOS) storage well, the basic element in a CCD

V_G

Metal gate

oxide

n^+

buried channel

pn junction

V_B

p-type substrate

Buried channel CCD
MOS plus pn junction
Prevents trapping by surface states at the semiconductor-oxide interface
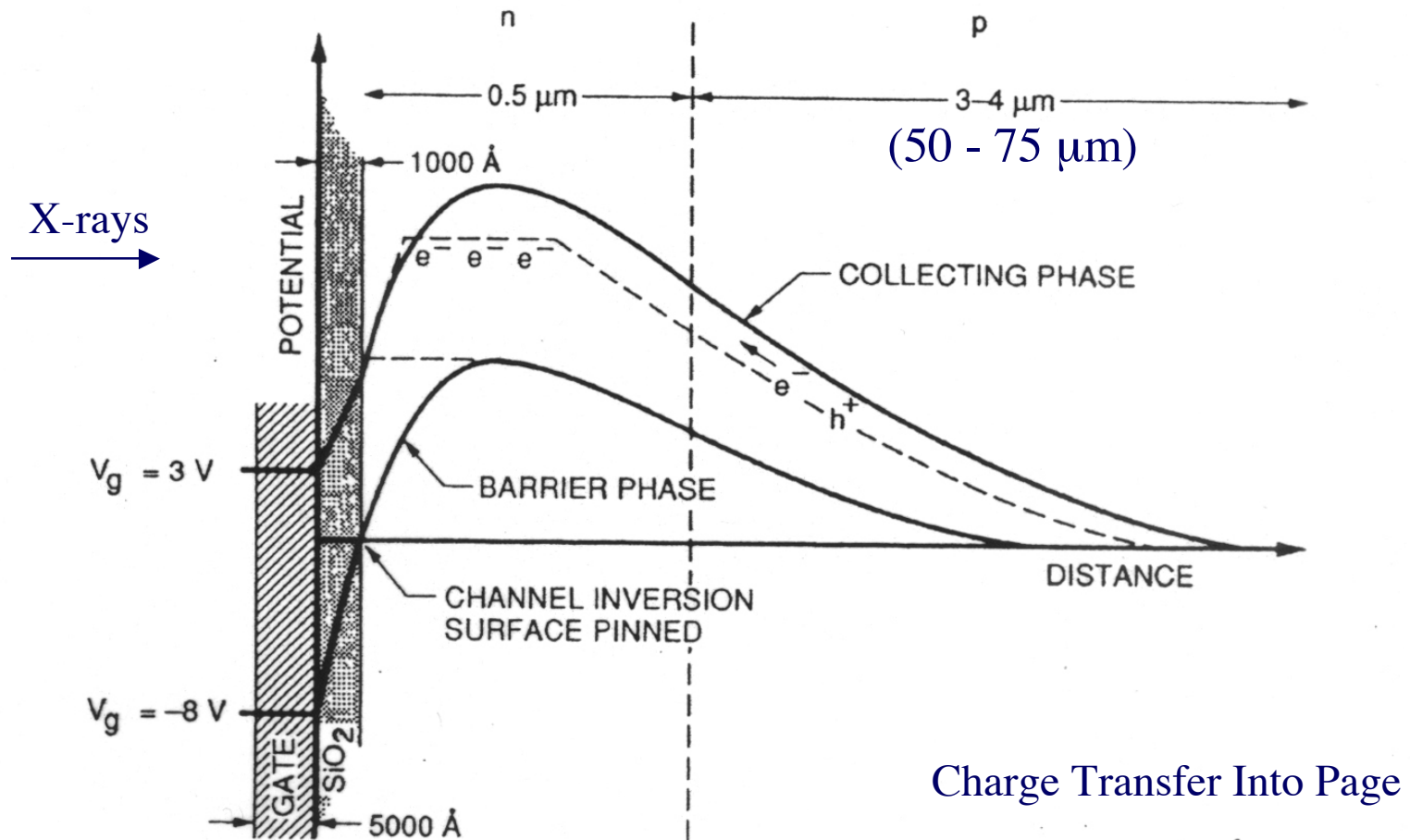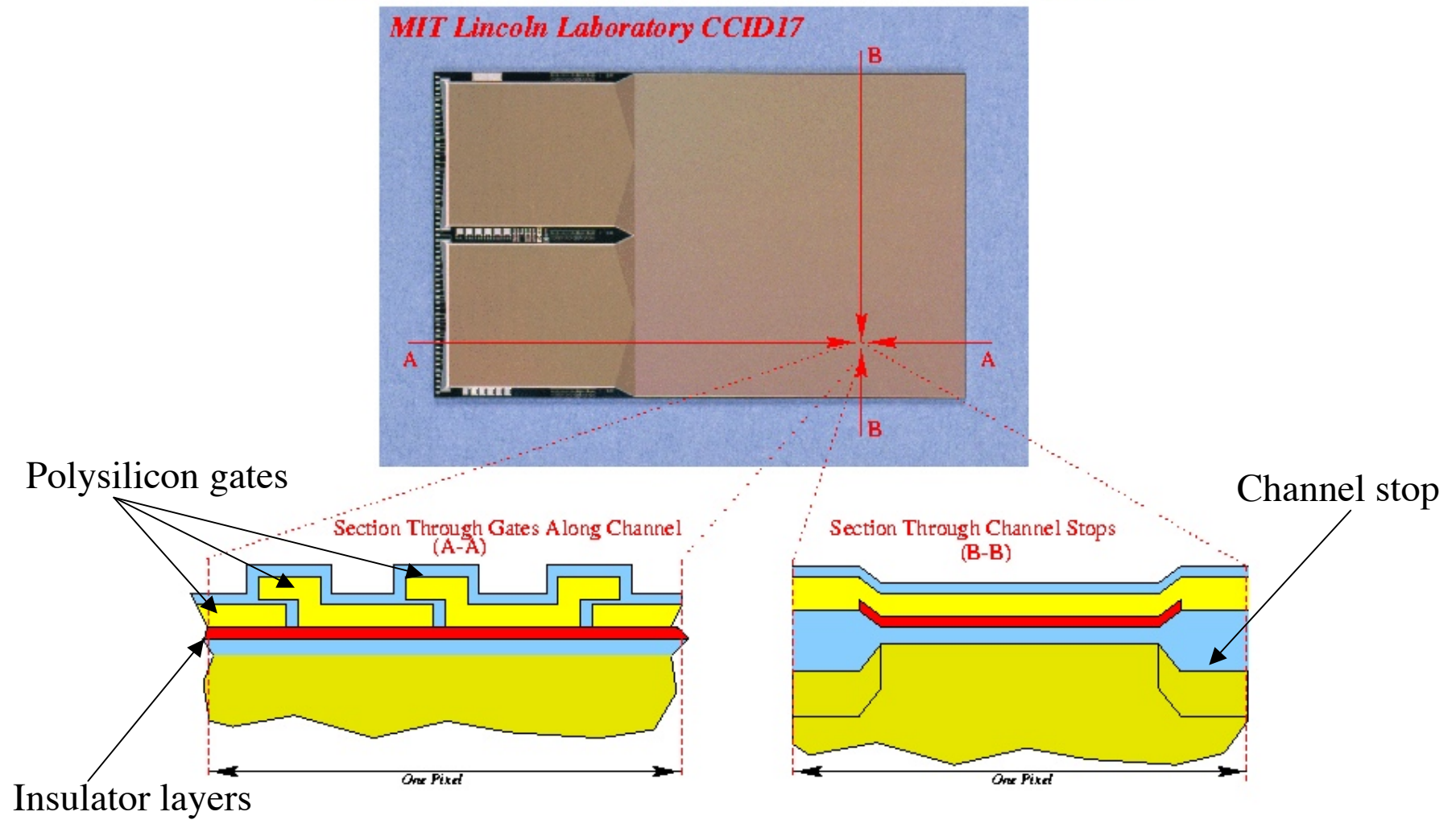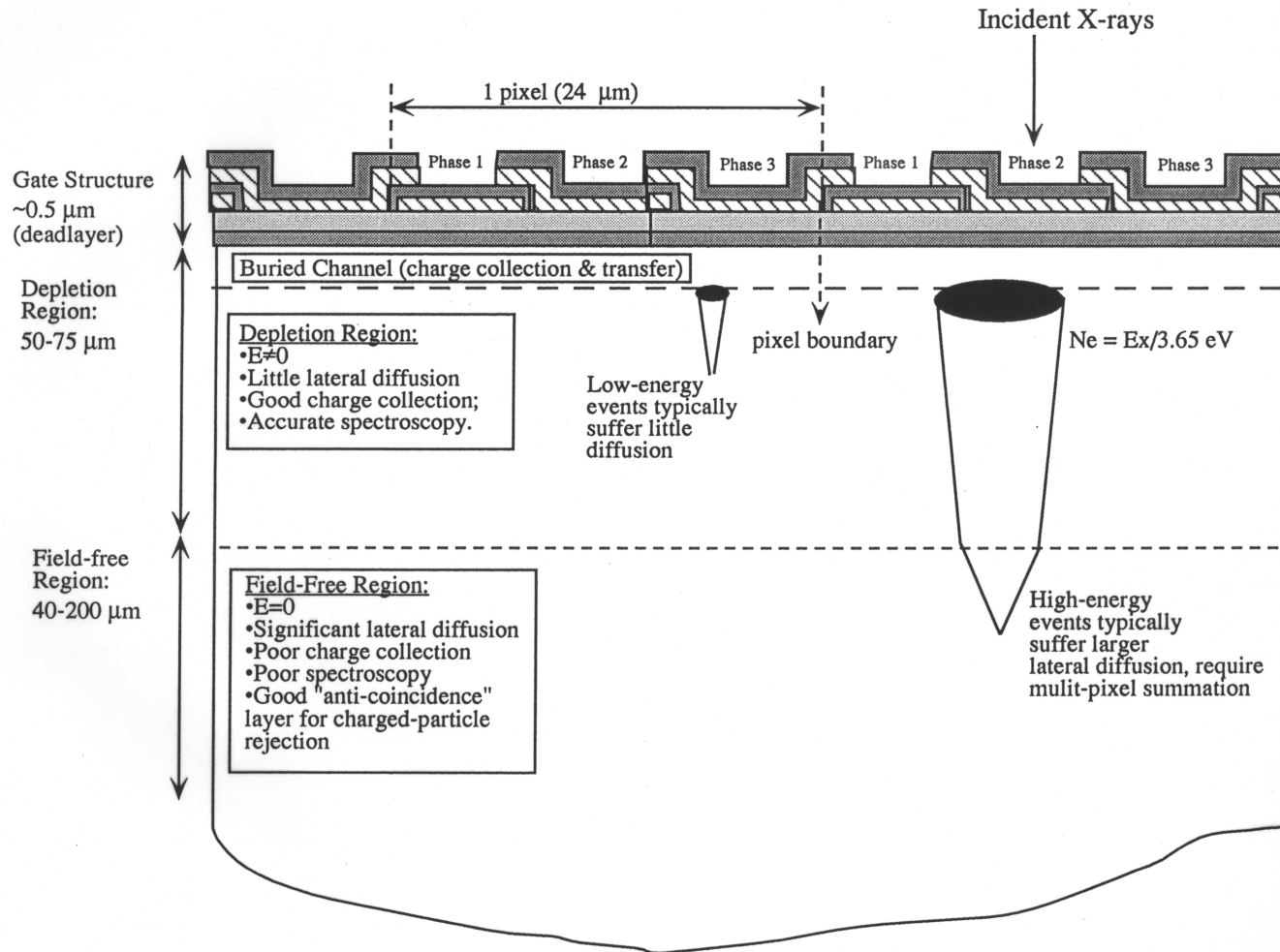
Electrostatic Potential in CCD

X-rays

Figure 1.19 Buried-channel potential well.

Charge Transfer Into Page

Janesick, 2001

Pixel Structure

Polysilicon gates

Channel stop

Insulator layers

Front-Illuminated X-ray CCD Structure
(not to scale)

Incident X-rays

1 pixel (24 μm)

Phase 1 | Phase 2 | Phase 3 | Phase 1 | Phase 2 | Phase 3

Gate Structure
~0.5 μm
(deadlayer)

Buried Channel (charge collection & transfer)

Depletion
Region:
50-75 μm

Depletion Region:
•E≠0
•Little lateral diffusion
•Good charge collection;
•Accurate spectroscopy.

pixel boundary

$Ne = Ex/3.65$ eV

Low-energy
events typically
suffer little
diffusion

Field-free
Region:
40-200 μm

Field-Free Region:
•E=0
•Significant lateral diffusion
•Poor charge collection
•Poor spectroscopy
•Good "anti-coincidence"
layer for charged-particle
rejection

High-energy
events typically
suffer larger
lateral diffusion, require
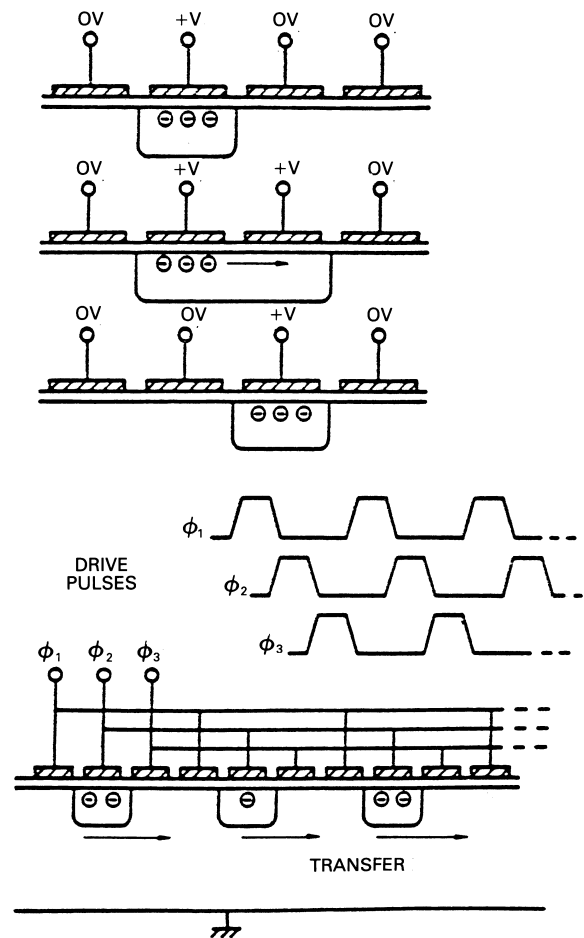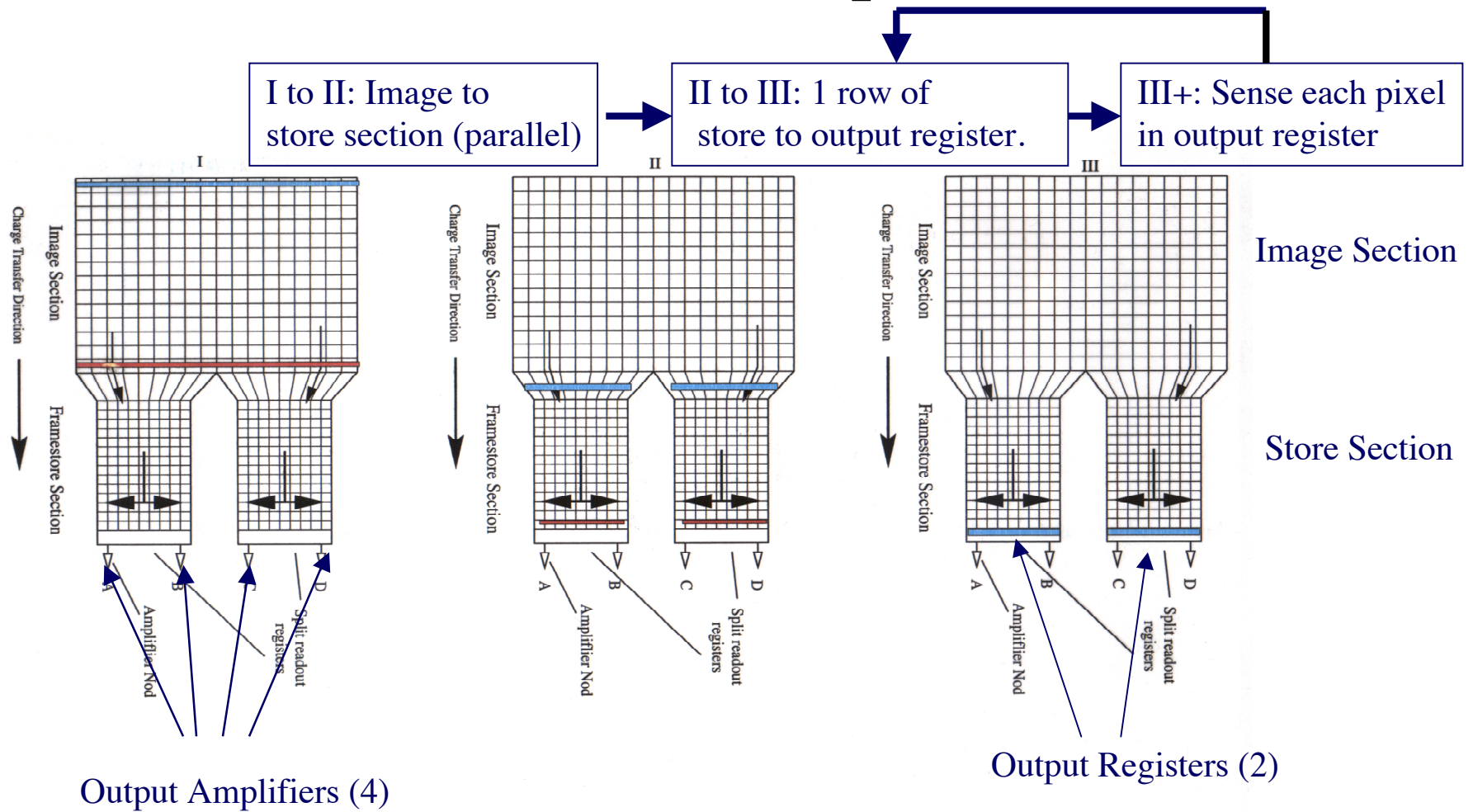mulit-pixel summation

CCD Charge Transfer

Fig. 6.9. Charge-coupling in a three-phase CCD and the associated timing waveform or clock pattern. In practice the degree of overlap between one electrode and the next depends on the CCD design.
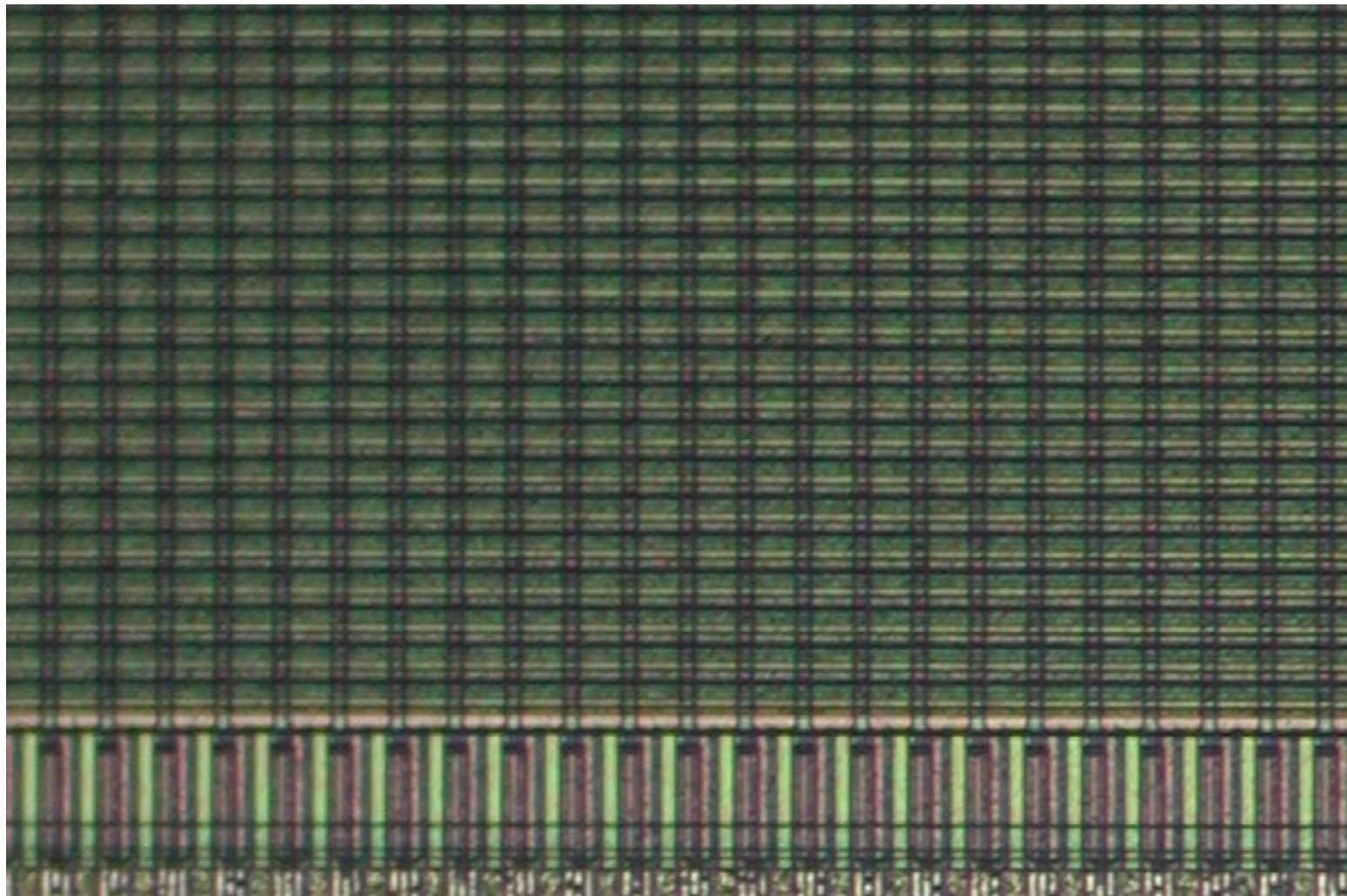
CCD Readout Sequence

I to II: Image to store section (parallel)	II to III: 1 row of store to output register.	III+: Sense each pixel in output register

Image Section

Store Section

Output Registers (2)

Output Amplifiers (4)

Charge Transfer Direction

Image Section

Framestore Section

Amplifier Nod

Split readout registers

# Front-illuminated CCD Gate Structure

21 μm-wide
framestore column

Overlapping
Gates

Output
Register

To Output

CCD Operating Modes

- X-ray CCDs operated in photon-counting mode
- Spectroscopy requires ≤ 1 photon interaction per pixel per frametime
- Minimum frametime limited by readout rate
- Tradeoff between increasing readout rate and noise
- For ACIS, 100 kHz readout $\Rightarrow$ 3.2 s frametime
- Frametime can be reduced by reading out subarrays or by continuous parallel clocking (1D imaging)
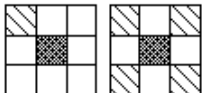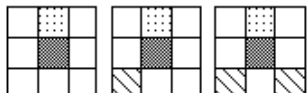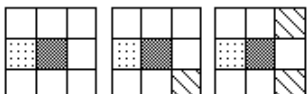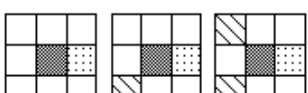

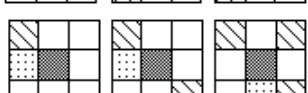|		
1/2	1/4	1/8
1.5 s	0.8 s	0.4 s
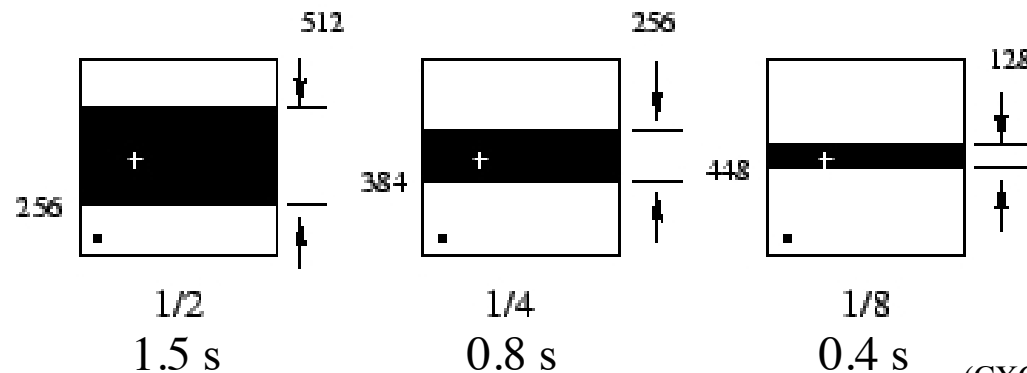
(CXC Proposer's Observatory Guide)

Event Processing

- CCD output rate (~10 Mbits/sec/CCD) exceeds telemetry resources
  - Raw CCD frames must be processed on-board to find prospective X-ray events
- Event selection:
  - CCD bias level determined and removed
  - Pixel pulseheight greater than threshold value ("event threshold")
  - Pixel is a local maximum (3 x 3 pixels on ACIS)
- For each event, record position, time and pulseheights of event island (3 x 3 pixels for ACIS)
- Events are assigned a grade which characterizes the shape of the event.

Grading Events

Grade definition — examples

✓ S = Perfect Single (Grade 0)

S+ = S + Detouched Corners (Grade 1)

✓ V = Vertical Single-Sided Split + Detouched Corners (Grade 2)

✓ L = Left Single-Sided Split + Detouched Corners (Grade 3)

✓ R = Right Single-Sided Split + Detouched Corners (Grade 4)

P+ = Single-Sided Split with Touched Corners (Grade 5)

✓ L+Q = L Shape and Square Shape + Detouched Corners (Grade 6)

Grade 7 - everything else

- A maximum level pixel larger than an event threshold
- A pixel larger than a split threshold which is included for the pulse height computation
- A pixel larger than a split threshold which is not included for the pulse height computation

- Event grade can be used to discriminate between X-ray and cosmic ray events
- In general, X-ray events split into simpler/smaller shapes (single, singly-split) ✓
- Cosmic ray events are more complex
- ASCA code grades are one example
- Onboard grade filtering can further reduce telemetry
- Grade filtering can improve spectral resolution - split events are noisier than singles

ACIS X-ray/Particle Discrimination
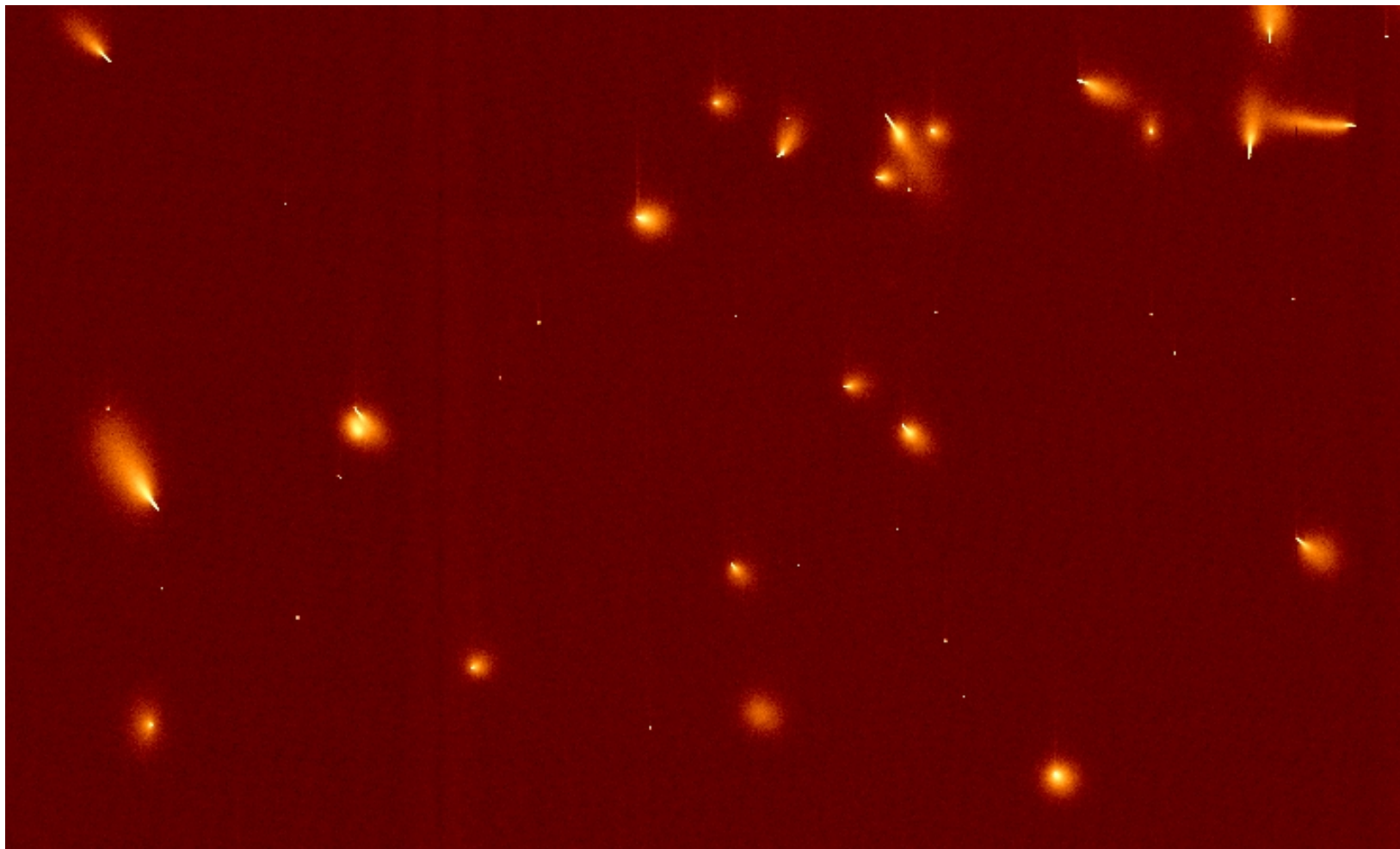
Blobs/streaks - charged particles.   Small dots - X-ray events.

CCD Quantum Efficiency
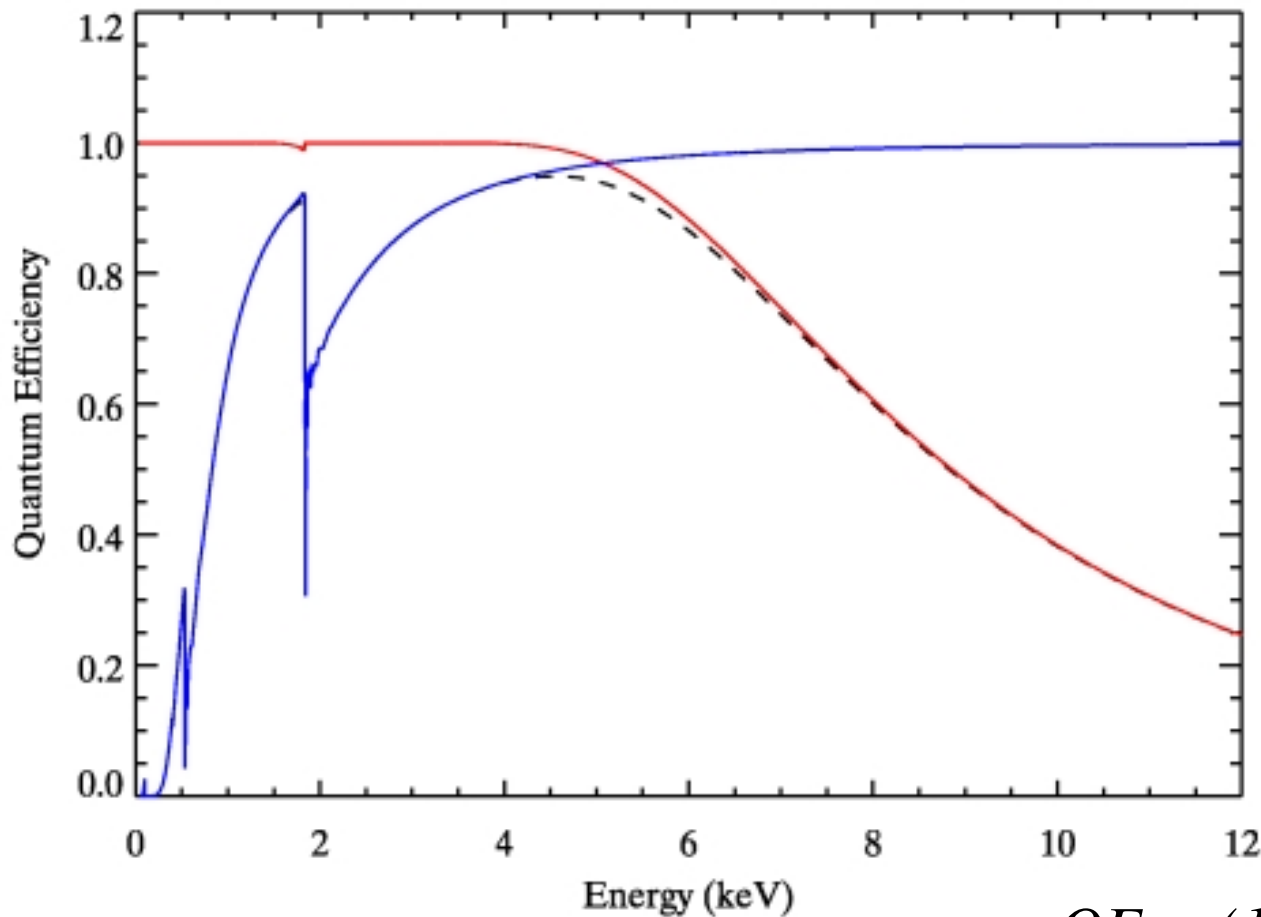
Transmission through deadlayers (channel stops, gates, oxide layers)

$$T = \Pi_i\, e^{-\mu_i t_i}$$

Absorption in depleted region

$$A = 1 - e^{-\mu_{Si} d}$$

μ is linear absorption coefficient
t thickness of deadlayer
d depletion depth

$$QE = (1 - e^{-\mu_{Si} d})\ \Pi_i\, e^{-\mu_i t_i}$$
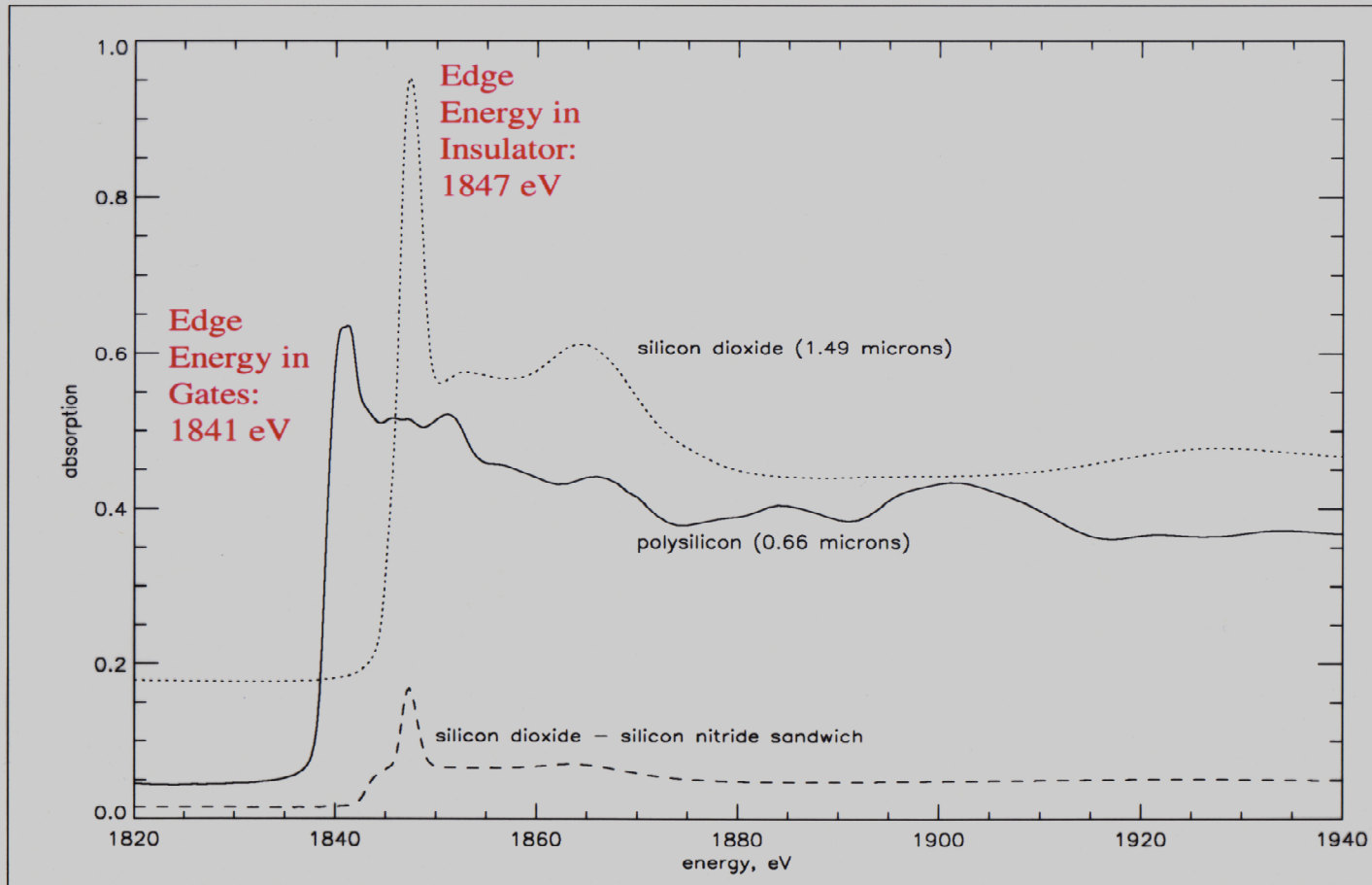
EXAFS - extended X-ray absorption fine structure

Optical Blocking Filters
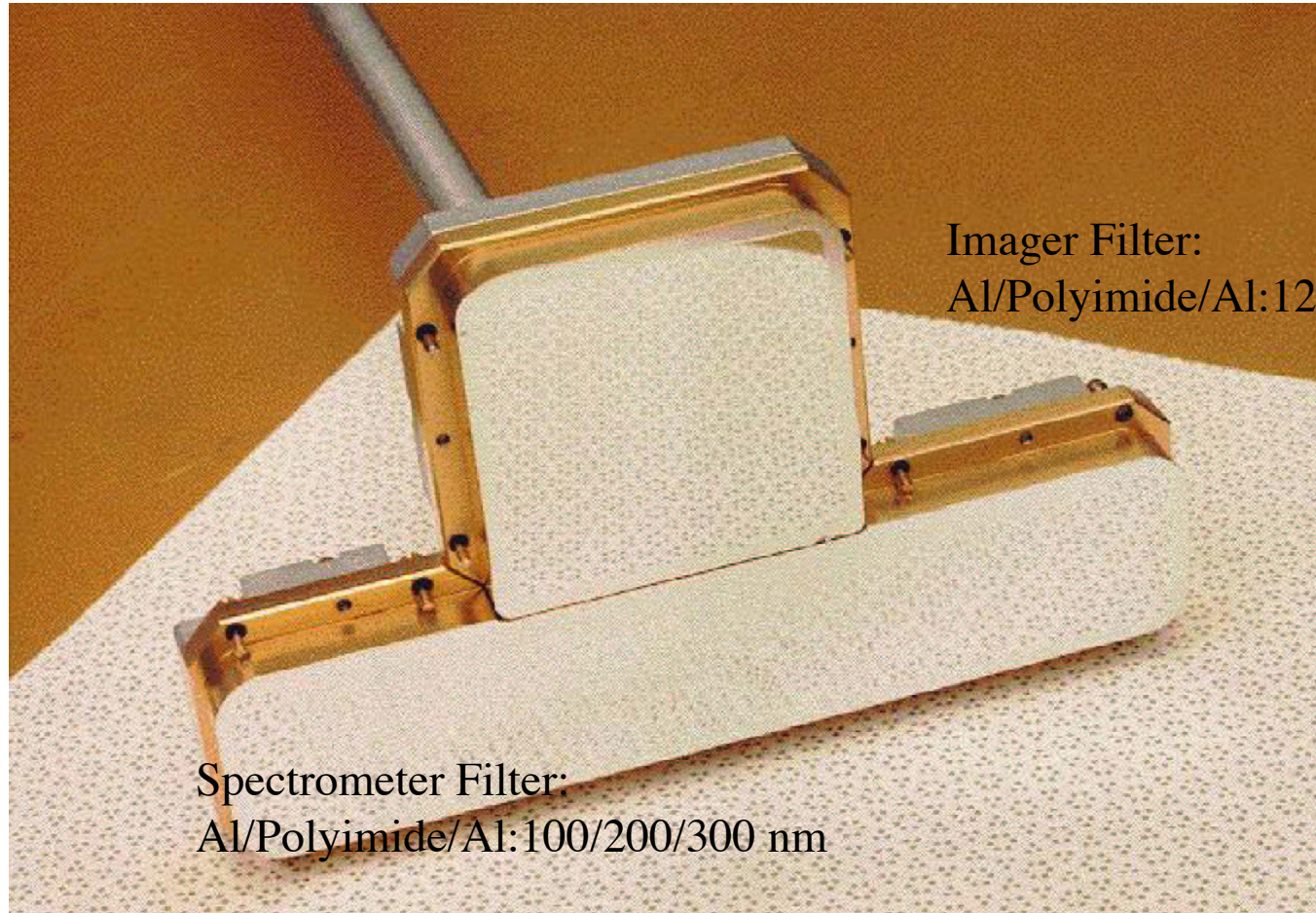
Imager Filter:
Al/Polyimide/Al:120/200/40 nm

Spectrometer Filter:
Al/Polyimide/Al:100/200/300 nm

- CCDs sensitive to optical photons
- Cause noise and pulseheight calibration issues
- Filter materials usually plastic and aluminum

Filter Transmission

At low energies (< 0.5 keV), > 50% reduction in efficiency

CCD X-ray Spectroscopy: The Basic Idea

- Photoelectric interaction of a single X-ray photon with a Si atom produces "free" electrons:

$$N_e = E_X / w \; (w \approx 3.7 \text{ eV}/e^-)$$

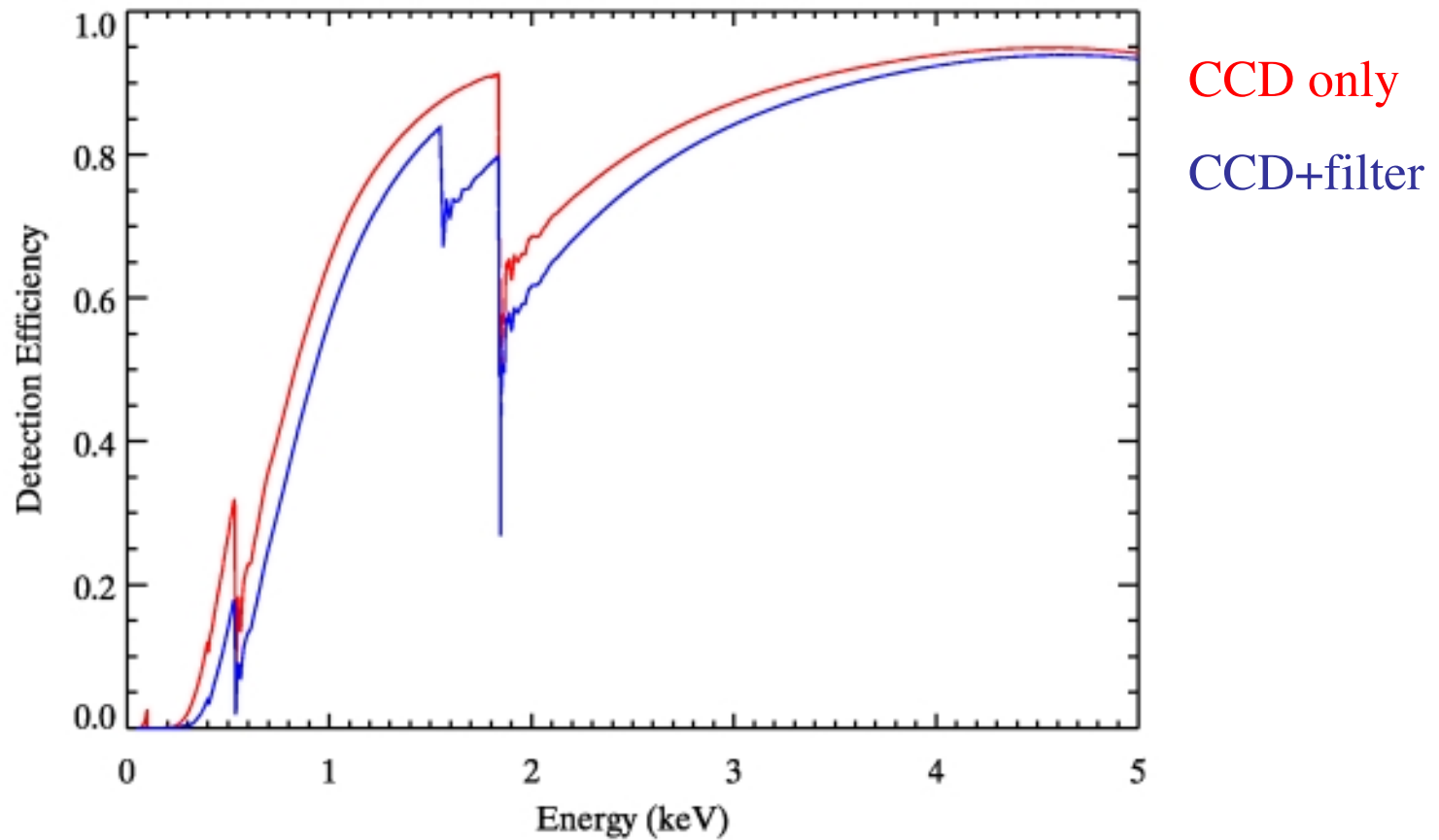$$\sigma_e^2 = F \times N_e \; (F \approx 0.12; \text{ not a Poisson process})$$

- Spectral resolution depends on CCD readout noise and physics of secondary ionization:

$$\text{FWHM (eV)} = 2.35 \times w \times \sqrt{\sigma_e^2 + \sigma_{read}^2}$$

- CCD characteristics that maximize spectral resolution:
  - Good charge collection and transfer efficiencies at very low signal levels
  - Low readout and dark-current noise (low operating temperature)
  - High readout rate (requires tradeoff vs. noise)

CCD X-ray Energy Resolution

- noise-free detector
- 4 e⁻ RMS readout noise
- 6 e⁻ RMS readout noise

ASCA SIS (1993): 4 e⁻ RMS
Chandra ACIS (1999): 2 e⁻ RMS
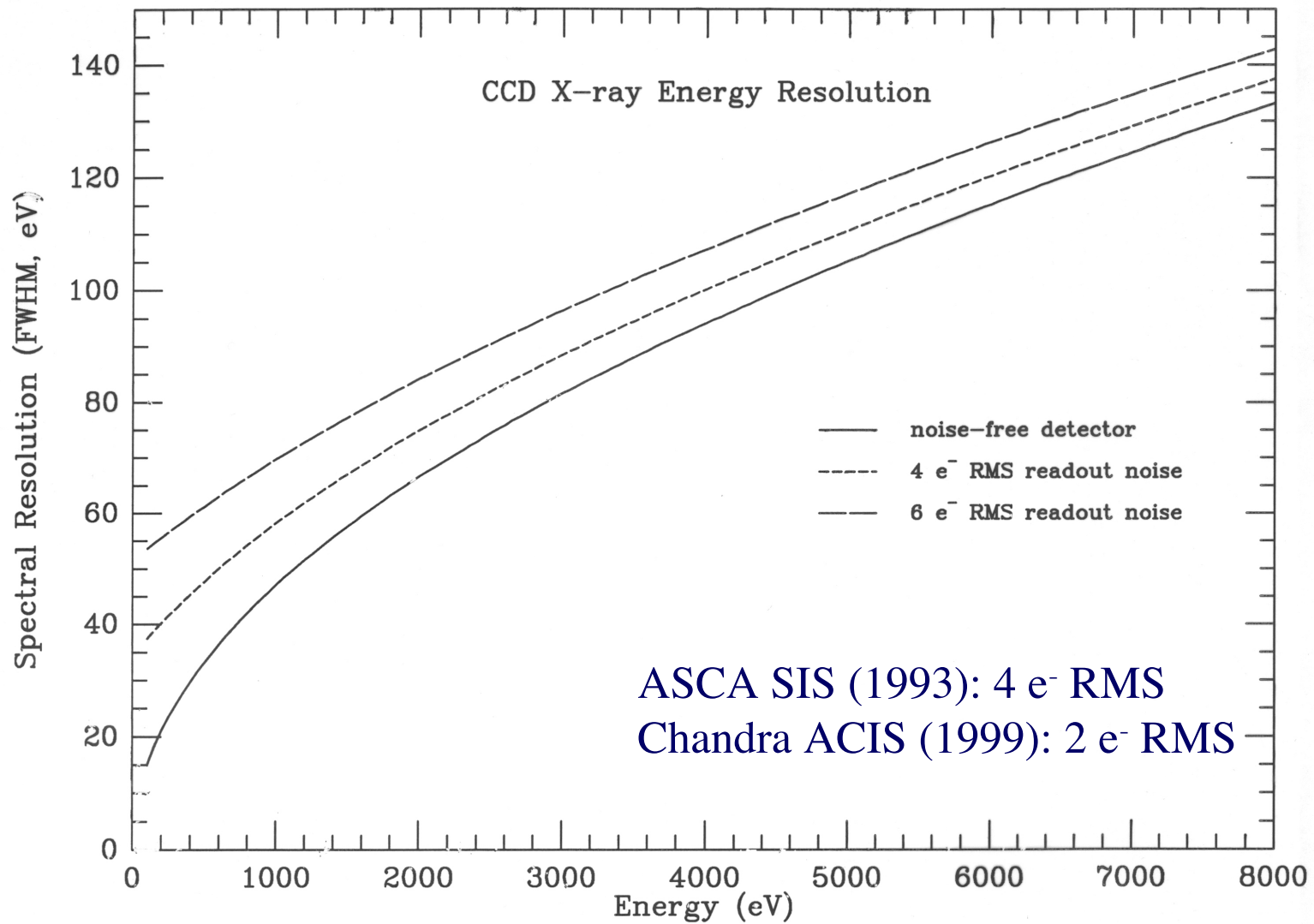
Spectral Redistribution Function
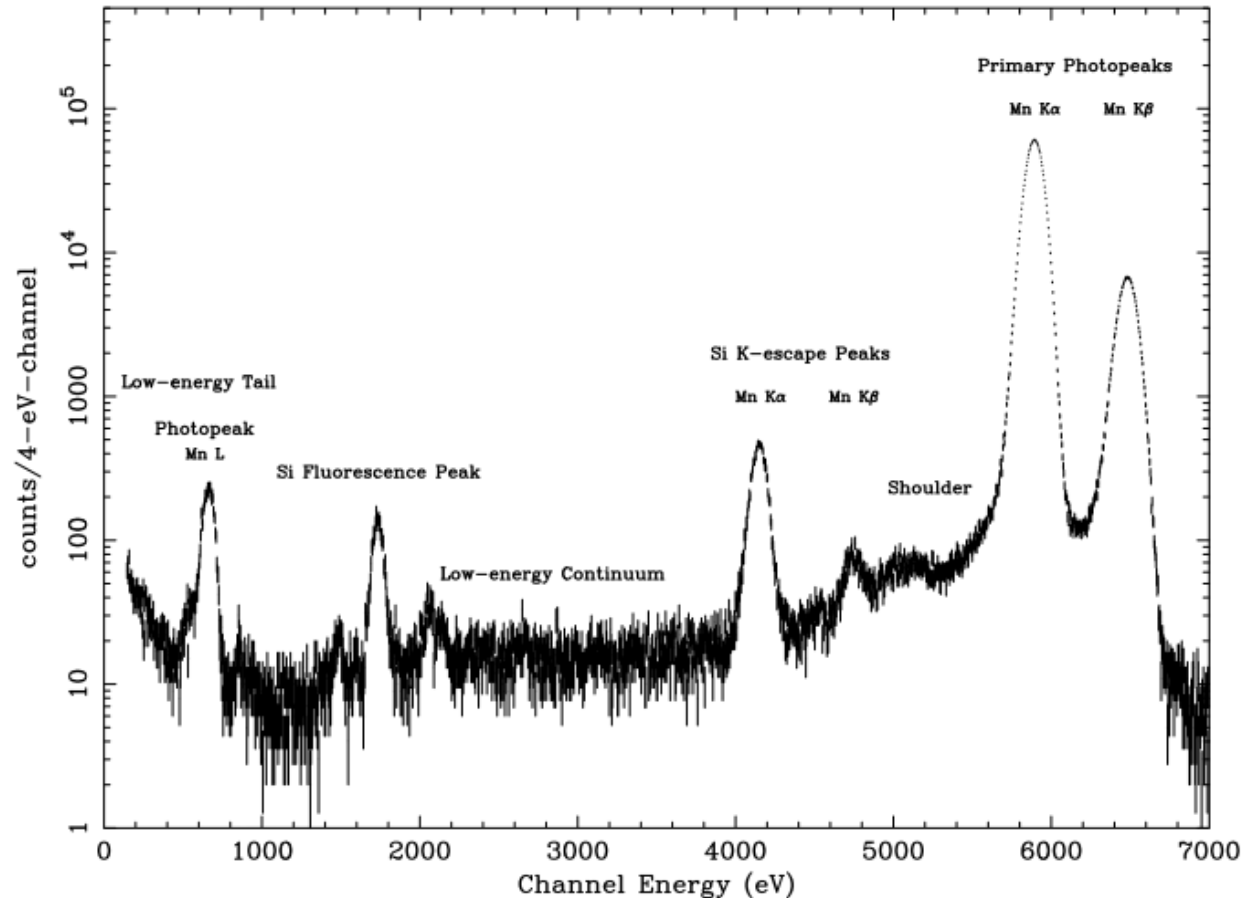
- Input spectrum has three spectral lines: Mn-L (0.7 keV), Mn-Kα (5.9 keV), and Mn-Kβ (6.4 keV)
- Instrument produces Si-K fluorescence and escape peaks, low-energy features
- Off nominal features ~2% of total

Schematic of Tail Model

Polysilicon gate

Gate insulator

Depleted silicon

Electron Cloud Sphere

Histogram of Events (log)

Energy

Low Energy Peak

Low Energy Tail

Main Peak
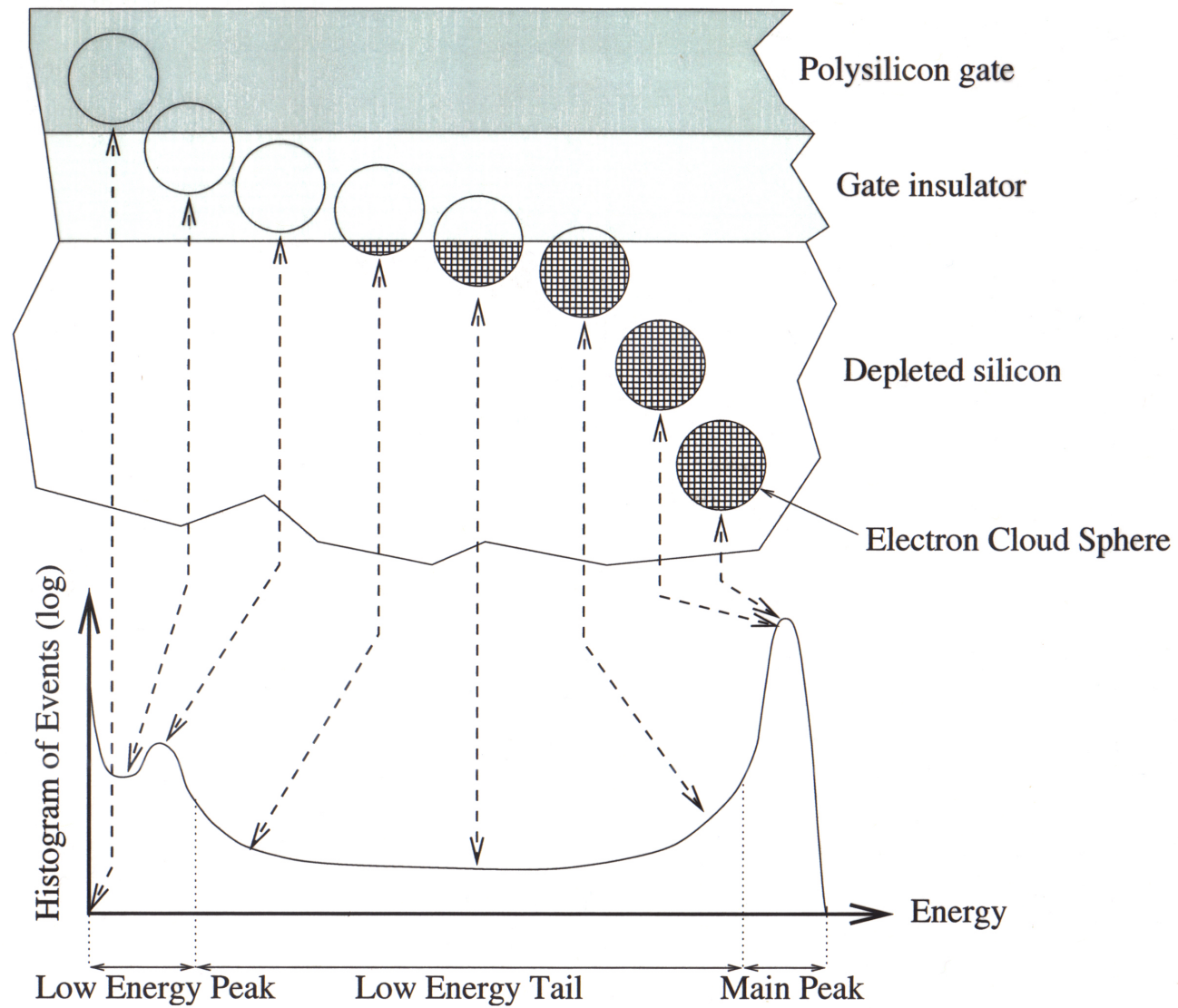
Low-Energy Detection Efficiency

- Many astrophysically interesting problems require good low-energy (< 1 keV) efficiency (pulsars, ISM absorption, SNR, …)

- Low energy X-rays are lost to absorption in gate structures and filter

- Solutions:
  – Thinned gates, open gates (XMM EPIC-MOS, Swift)
  – Back-illumination (Chandra ACIS, XMM EPIC-PN, Suzaku XIS)

Back-illuminated CCDs

FRONT ILLUMINATED WAFER

THIN (Except for rim support)

BACK SURFACE TREATMENT

SiO$_2$

p$^+$

SiO$_2$ (35 nm) p$^+$ (~50 nm)

poly

HIGH RESISTIVITY p-Si   n V_G

~ 40 μm

hv
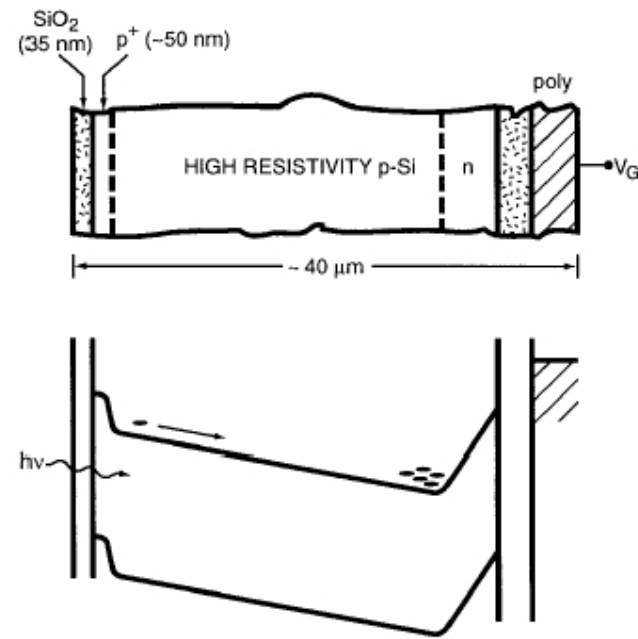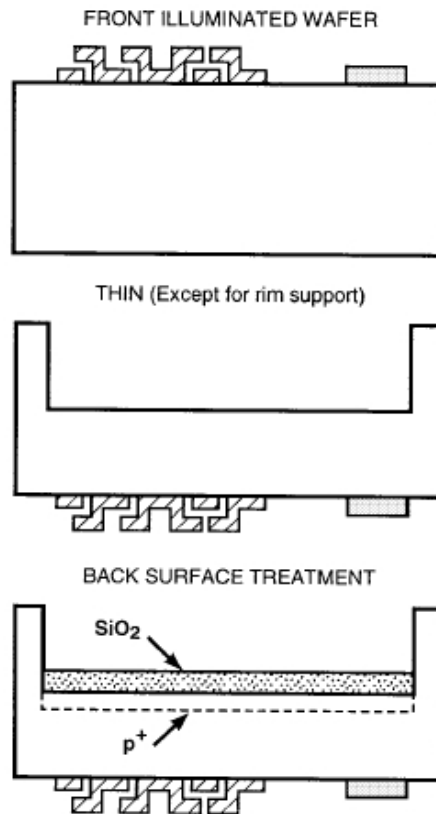
Burke et al., 1997, IEEE Trans. on EE, 44, 1633

- Front-illuminated CCD, reversed and thinned
- Gates structures and channel stops are not deadlayers

Back-illuminated CCDs

- Thinner deadlayers $\Rightarrow$ higher low-E QE
- Thinner active region $\Rightarrow$ lower high-E QE
- Increased noise, charge transfer inefficiency $\Rightarrow$ higher FWHM

First Readout of ACIS CCDs

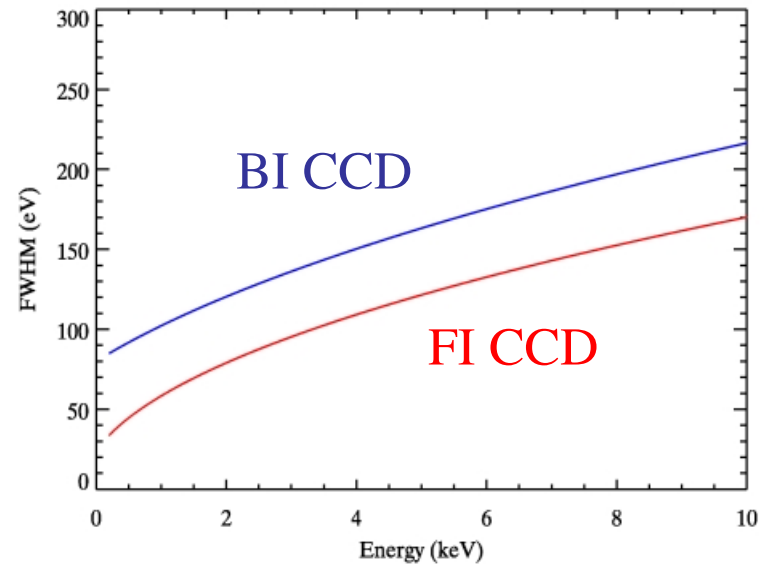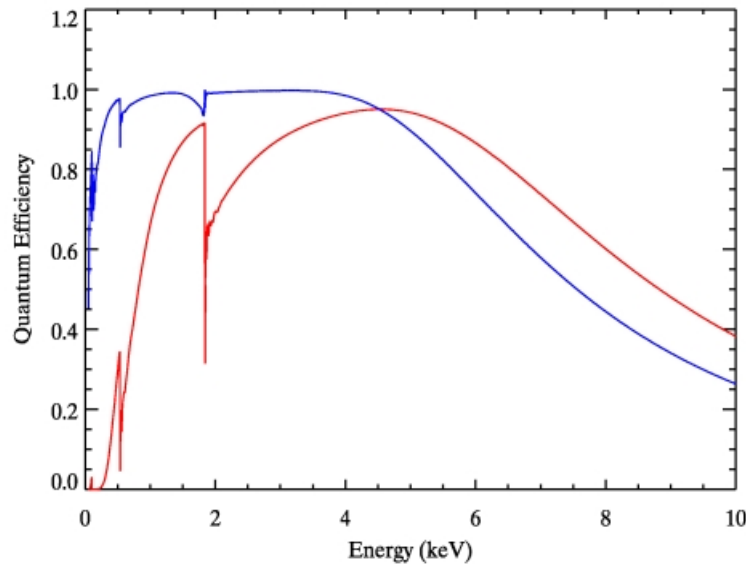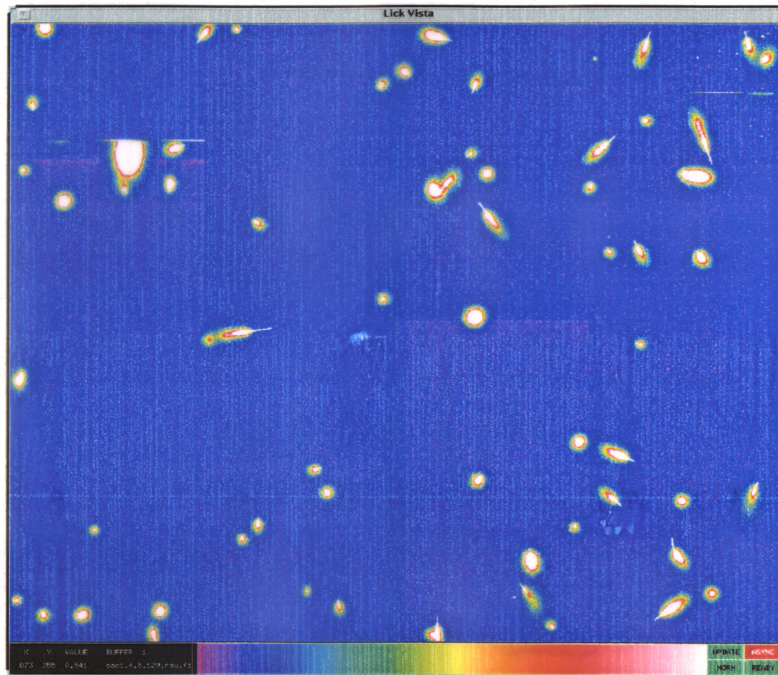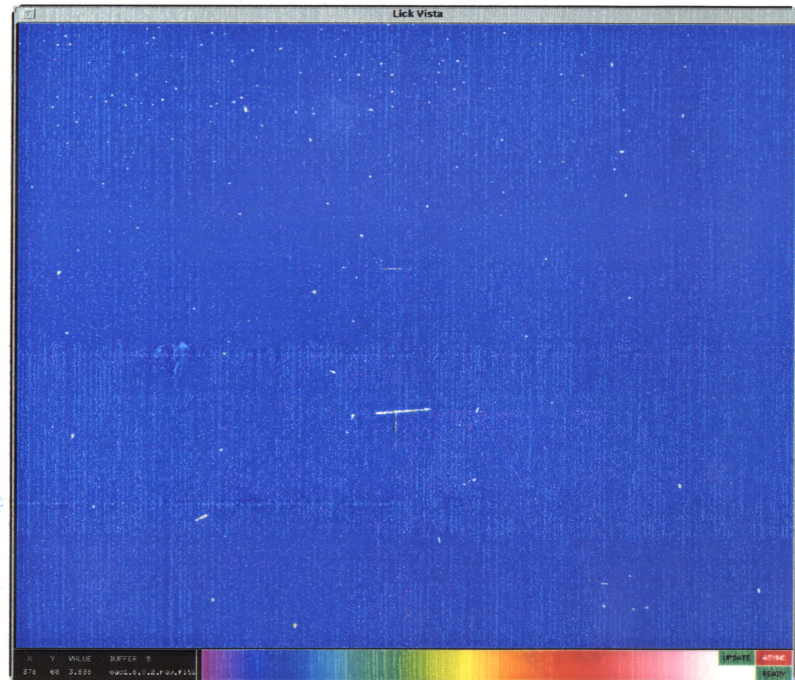S2 = w182c4r

S3 = w134c4r

We first read charge from the ACIS CCD detectors on-orbit on July 27, 1999 at about 8:25pm local (EDT) time (209:01515Z). At this point the ACIS door was still closed and Chandra was not yet in its final orbit. The focal plane temperature was -90C. An an altitude of about 60,000km, we were greeted by a host of cosmic-ray and other particle tracks. The undepleted bulk of the front-illuminated device at focal plane position S2 (ccid17-182-4r) causes large and interesting particle tracks, especially when the interaction occurs in the framestore (the output register is at the top in these pictures.) The response of the thinner (40-micron-thick) back-illuminated chip at S3 (ccid17-134-4r) is much less alarming, but in the end the background rejection efficiency of the FI devices is better by a factor of 3. Some X-ray events from the ACIS Internal Calibration Source are visible at the top of the S3 image. For all 10 devices on the focal plane, the readout noise, as measured from the overclocked pixels, was found to be 2-3 electrons, RMS, just as it was on the ground. Exposure time for these images is about 3.3 seconds.

Characteristics of Some "Current Generation" X-ray CCDs

Characteristic	Chandra-ACIS		XMM-Newton-EPIC	
	FI	BI	MOS	PN
Electrode Technology	3-poly MOS	3-poly MOS	3-poly MOS (open electrode)	Junction
Illumination	Front	Back	Front	Back
Pixel Size (μm)	24	24	40	150
Format	1k x 1k	1k x 1k	600 x 600	200 x 64
Detectors in Focal Plane	8	2	2 x 7	12
Focal Plane Sensitive Area (cm^2)	48 + 12		2 x 40	35
System Noise (e$^-$, RMS)	2	3	5	5
Single Channel Readout Rate (kpix s^{-1})	100	100	128	43
Readout Channels per Detector	4	4	1	64 analog + 1 A/D
Full Focal Plane Frame Time (s)	3.2	3.2	2.8	0.074
Charge Transfer Inefficiency (Pre-flight)	$< 3 \times 10^{-6}$	$< 1 - 3 \times 10^{-5}$	$< 3 \times 10^{-6}$	$\sim 10^{-4}$
Depletion Depth (μm)	75	40	40	300
Energy Resolution (eV, FWHM):				
at 0.525 keV	45	100	>80	70
at 5.9 keV	135	150	135	135
CCD Manufacturer	MIT/Lincoln	MIT/Lincoln	MAT (EEV)	MPE/HLL

ASCA, HETE and Suzaku XIS similar to ACIS
Swift similar to EPIC-MOS

Chandra ACIS Focal Plane
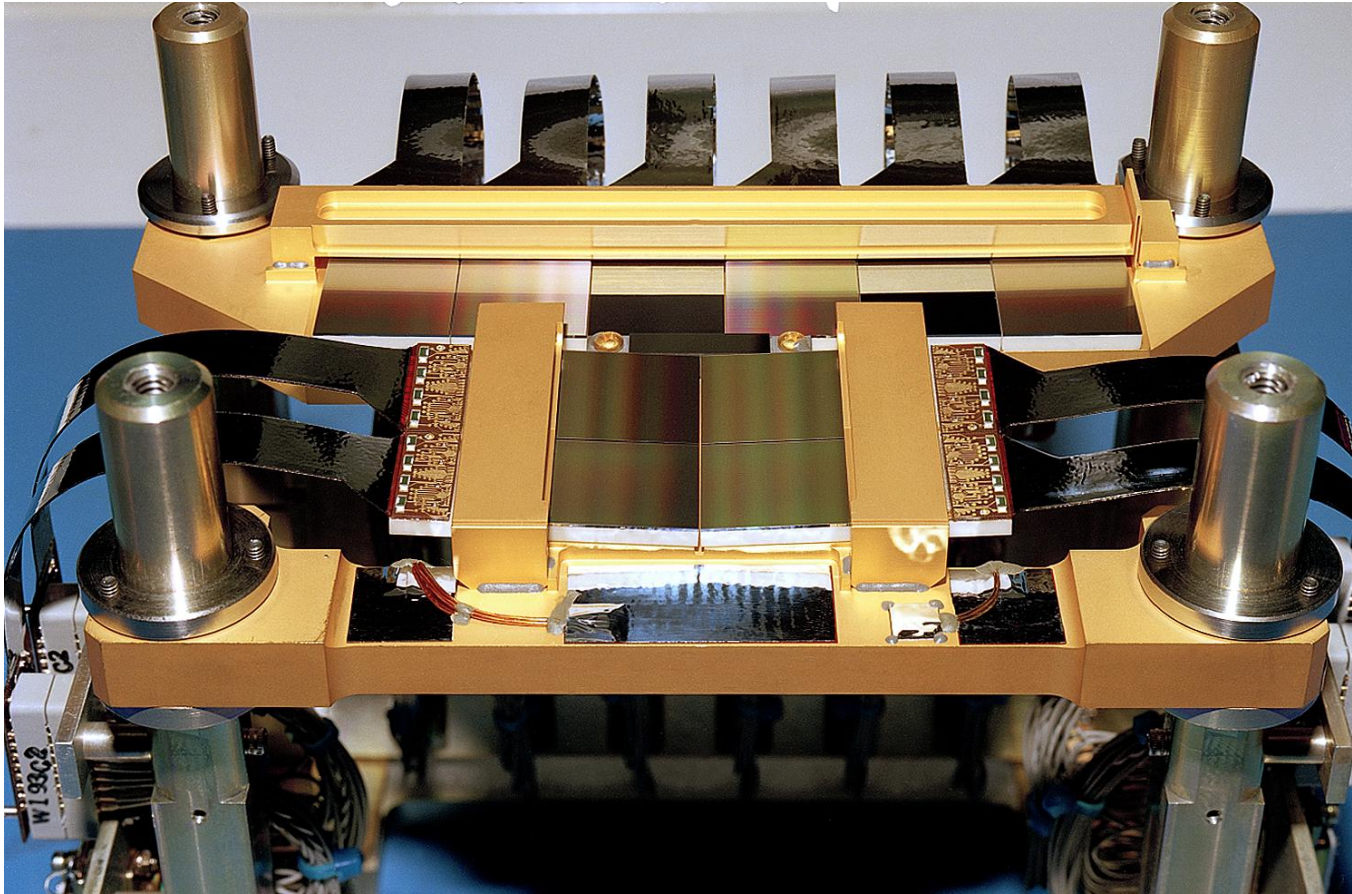
The Advanced CCD Imaging Spectrometer (ACIS) contains 10 planar, 1024 x 1024 pixel CCDs ; four arranged in a 2x2 array (ACIS-I) used for imaging, and six arranged in a 1x6 array (ACIS-S) used either for imaging or as a grating readout. Two CCDs are back-illuminated (BI) and eight are front-illuminated (FI).

XMM-Newton EPIC-MOS
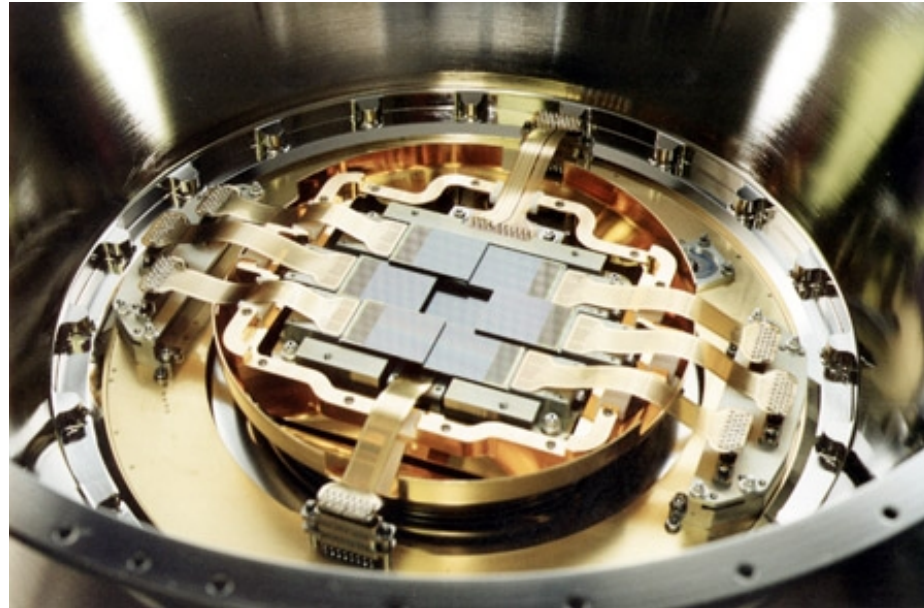
The MOS EEV CCD22 is a three-phase frame transfer device on high resistivity epitaxial silicon with an open-electrode structure; it has a useful quantum efficiency in the energy range 0.2 to 10 keV. The low energy response of the conventional front illuminated CCD is poor below ~700 eV because of absorption in the electrode structure. For EPIC MOS, one of the three electrodes has been enlarged to occupy a greater fraction of each pixel, and holes have been etched through this enlarged electrode to the gate oxide. This gives an "open" fraction of the total pixel area of 40%; this region has a high transmission for very soft X-rays that would have otherwise be absorbed in the electrodes. In the etched areas, the surface potential is pinned to the substrate potential by means of "pinning implant". High energy efficiency is defined by the resistivity of the epitaxial silicon (around 400 Ohm-cm). The epitaxial layer is 80 microns thick (p-type). The actual mean depletion of the flight CCDs is between 35 to 40 microns: the open phase region is not fully depleted. Image and caption taken from http://xmm.vilspa.esa.es/external/xmm_user_support/documentation/technical/EPIC

XMM-Newton EPIC-PN
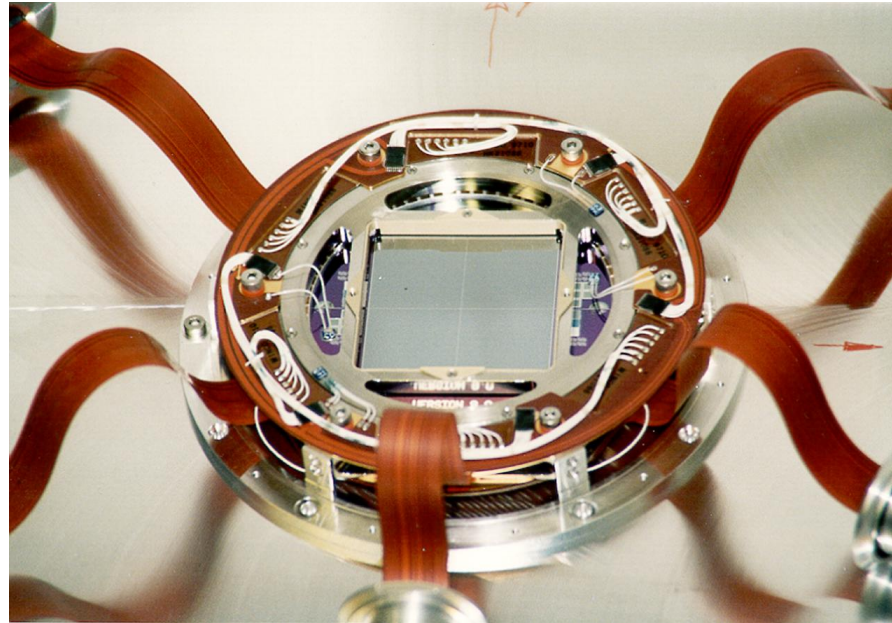
The PN-CCDs are back-illuminated. In the event of an X-ray interaction with the silicon atoms, electrons and holes are generated in numbers proportional to the energy of the incident photon. The average energy required to form an electron-hole pair is 3.7 eV at -90° C. The strong electric fields in the pn-CCD detector separate the electrons and holes before they recombine. Signal charges (in our case electrons), are drifted to the potential minimum and stored under the transfer registers. The positively charged holes move to the negatively biased back side, where they are 'absorbed'. The electrons, captured in the potential wells 10 microns below the surface can be transferred towards the readout nodes upon command, conserving the local charge distribution patterns from the ionization process. Each CCD line is terminated by a readout amplifier. The picture shows the twelve chips mounted and the connections to the integrated preamplifiers.

Photon Pileup

- If two or more photons interact within a few pixels of each other before the image is readout, the event finding algorithm may regard them as a single event
  - Increased amplitude
  - Reduction of detected events
  - Spectral hardening of continuum
  - Distortion of PSF
- Correcting for pile-up is complicated
- Best to set up observation to minimize pileup

Photon Pileup

Monochromatic Source

Detected event rate: 0.14 evts/frame

Bright

Detected event rate: 0.32 evts/frame

Brighter

Detected event rate: 1.34 evts/frame

Brightest

Counts/sec

Energy
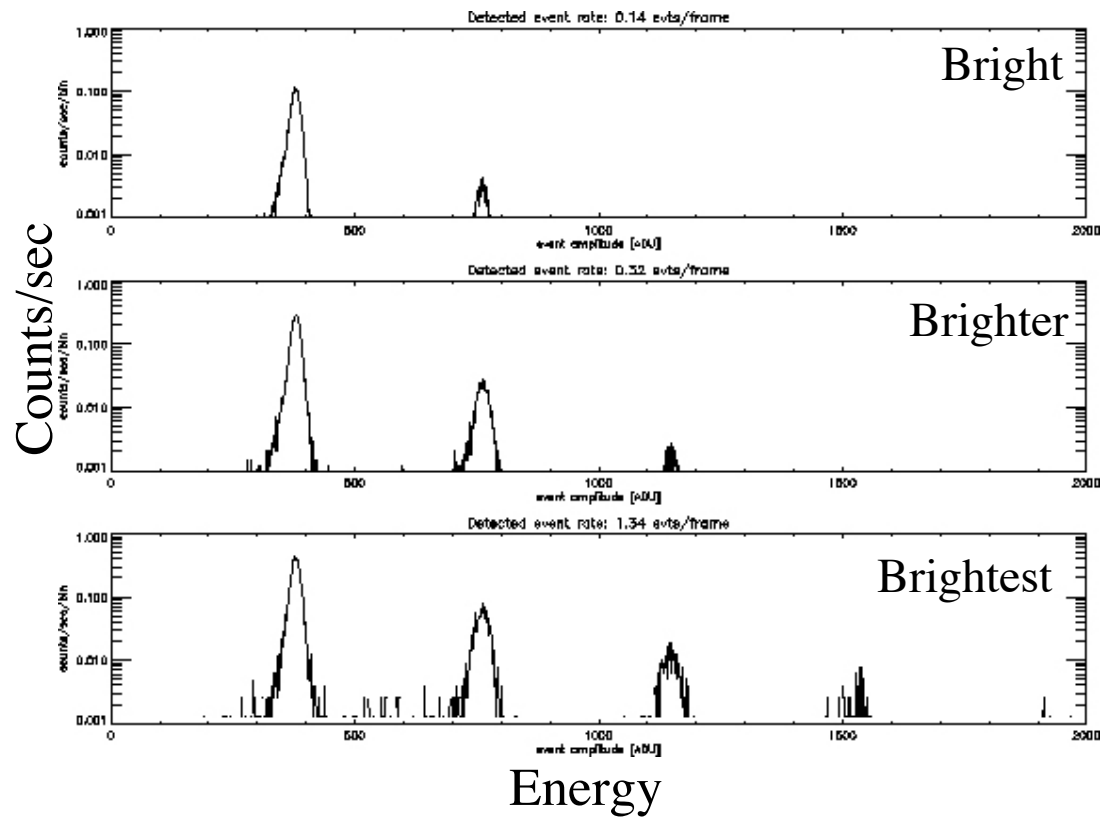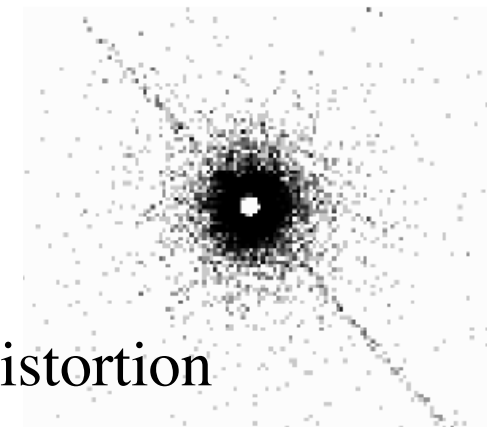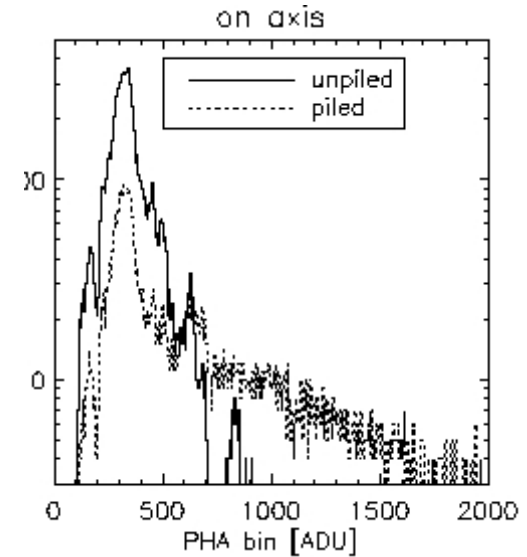
(From Chandra Proposer's Observatory Guide)

Thermal Spectrum

on axis

unpiled
piled

PHA bin [ADU]

PSF Distortion

Readout Streak/Out-of-time Events

3C273 - Quasar with jet

Transfer Direction
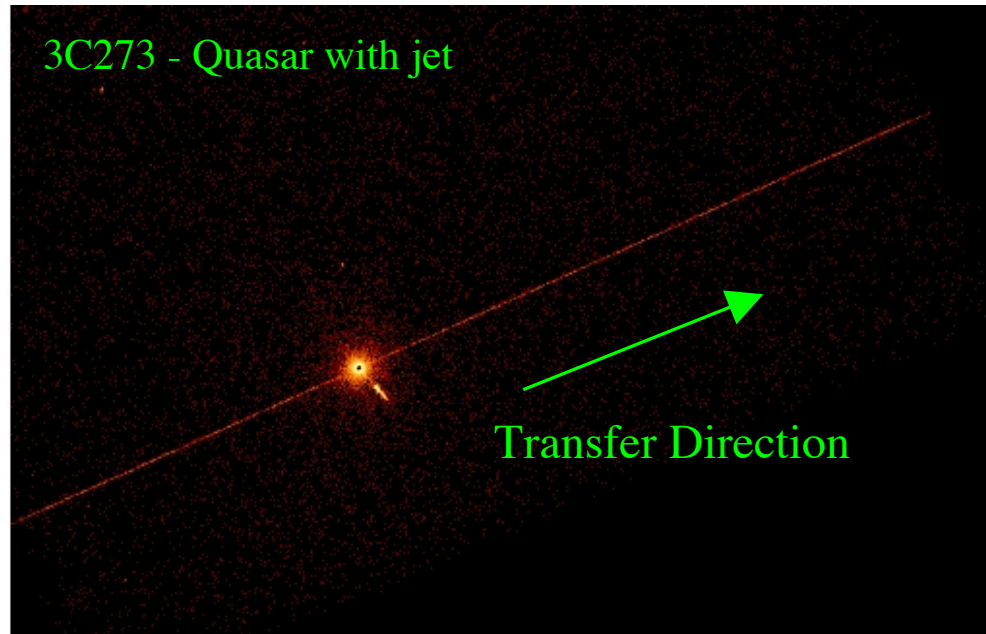
- Photons that interact while imaging array is transferring
- Assigned incorrect row/chip y value
  - Events may have poor initial calibration
- Can be modeled & removed
- Streak events have higher time resolution, no pileup

Charge Transfer Inefficiency

- X-ray events lose charge to charge trapping sites.
- Leads to:
  - Position dependent gain
  - Spectral resolution degradation
  - Position dependent QE
- Caused by radiation damage or manufacturing defects
- Depends on:
  - Density of charge trapping sites
  - Charge trap capture and re-emission properties (temperature)
  - Occupancy of charge traps (particle background)

ACIS-I3, Node 3, -120C, G02346
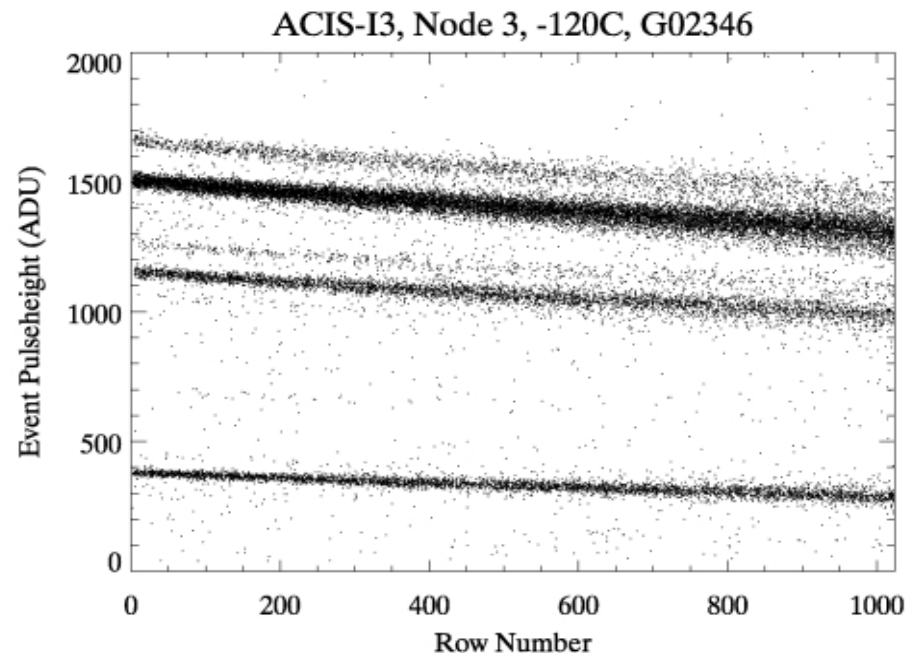
Physics of Radiation-induced Charge Transfer Inefficiency

- Photoelectrons (and secondary ionization) liberated by an incident X-ray are not really "free"; they occupy conduction band states.

- The existence of the conduction band depends on the symmetric arrangment of atoms in the lattice.

- When the lattice is damaged by incident particles (such as protons), its symmetry is disrupted.

- Electron "traps" (new, localized bound states) can be associated with radiation-induced lattice disruptions.

- If electrons encounter such traps during the readout process, they can be left behind, and thus lost from the X-ray induced charge packet. Eventually, trapped electrons can be released via thermal excitation.

- Since the loss process is stochastic, (especially in the presence of random background charged particle radiation) the traps degrade the spectral resolution.

Thermal Control and Contamination

- For best performance (reduced dark current and CTI), CCDs must be operated cold (−60C - −120C)

- Can use active (TEC) or passive (radiators) thermal control

- Often coldest surface, danger of contamination

- Contamination acts as an additional absorbing layer

ACIS-S3 Transmission at 700 eV
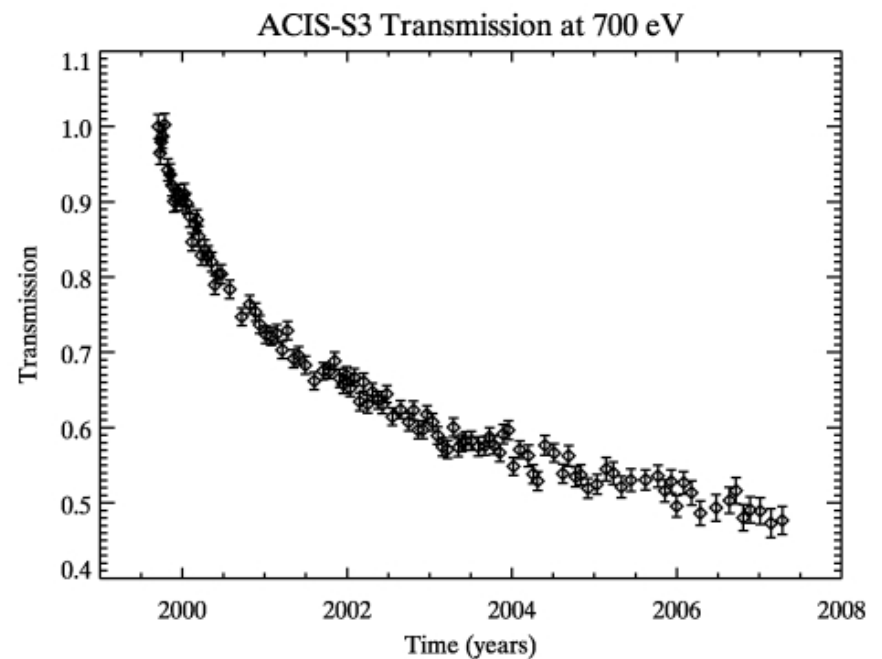
Spectrum of the Quiescent Background
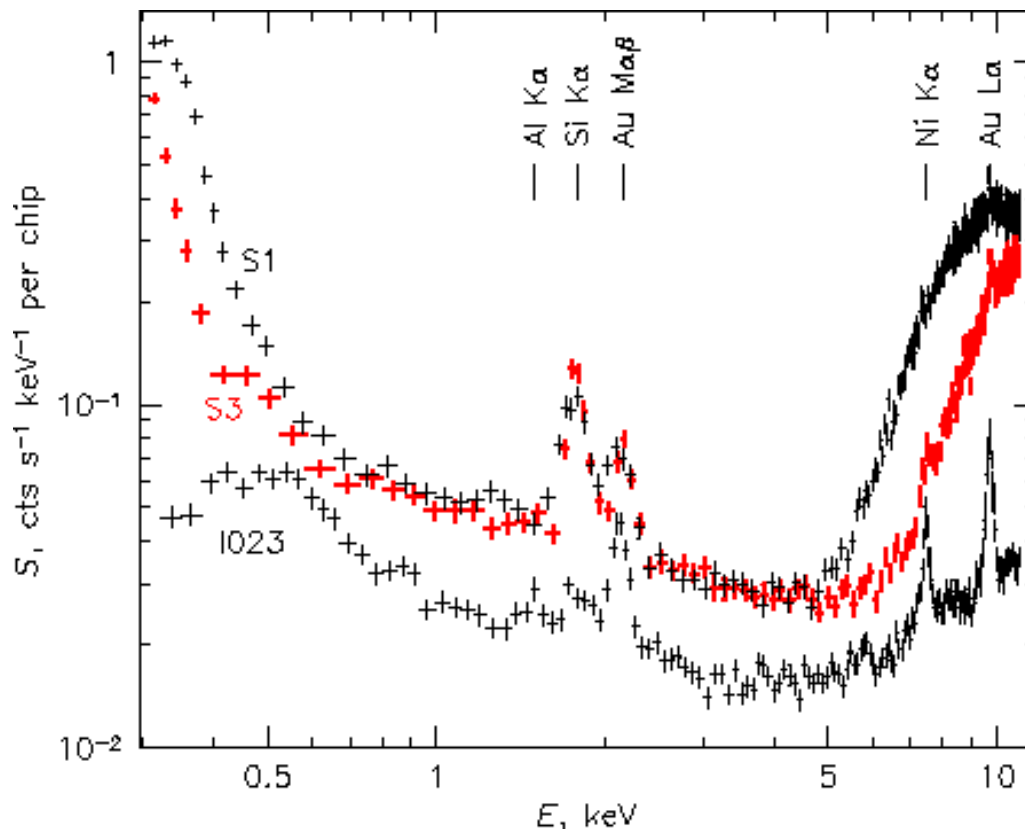
Spectra of the charged particle ACIS background with ACIS in the stowed position. Line features are due to fluorescence of material in the telescope and focal plane.
S1 and S3 are BI CCDs
I023 are FI CCDs

(CXC, Proposer's Observatory Guide)

- Cosmic-ray induced events plus soft diffuse cosmic X-ray background
- Background can be reduced by grade filtering
    -Less effective for back-illuminated CCDs
- Otherwise, background can be modeled or estimated and subtracted

Background Flaring

- Short-lived increases in background rate

- Usually low energy, effects BI more than FI

- Some correlation with solar flares and geomagnetic conditions

- Believed to be low energy (~100 keV) protons

- Not seen in low earth orbit
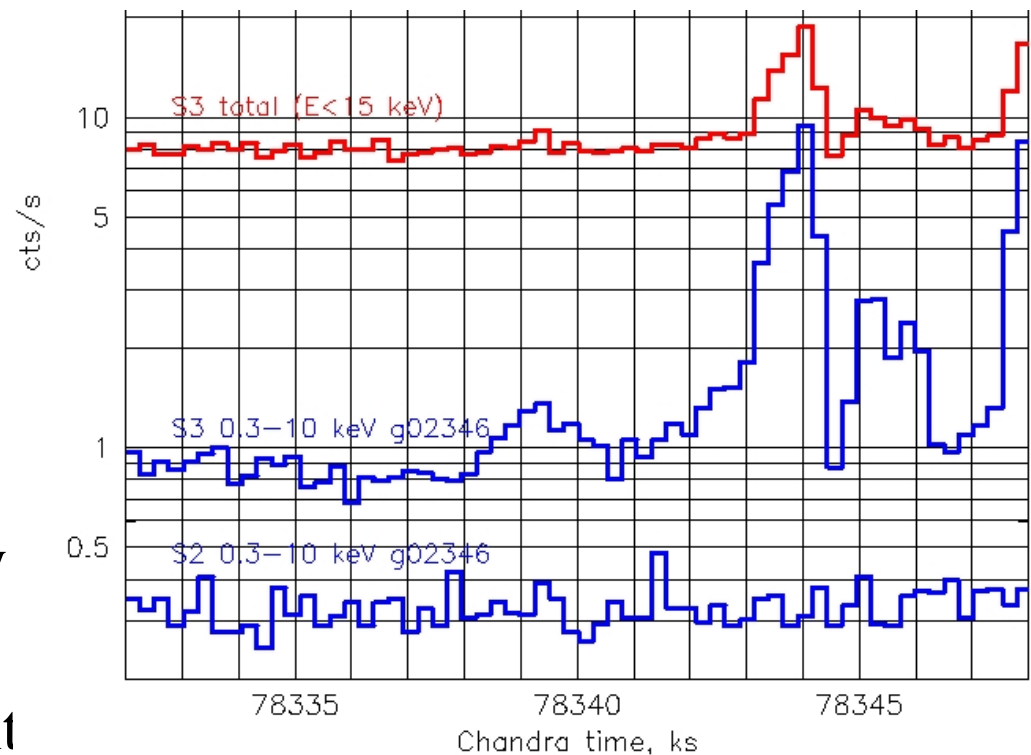
(Markevitch, CXC Calibration)

Hot Pixels, Flickering Pixels

- Radiation damage or manufacturing defects can cause pixels to have anomalously high dark current
- Can regularly exceed event threshold and cause spurious events
- Extreme cases may be removed onboard, otherwise filtered in data analysis
- Strongly correlated with temperature
  - More important for ASCA (–60C) and Suzaku (–90C) than ACIS (–120C)
- Unstable defects cause flickering pixels
  - Lower frequency, more difficult to detect and remove

Future X-ray Imaging Detectors

- Photon-counting X-ray CCDs in operation on five observatories (Chandra, XMM-Newton, HETE-2, Swift, Suzaku)

- Microcalorimeter detectors provide 10-20x improvement in spectral resolution but not megapixel imaging or good low energy QE (at least not yet)

- Megapixel imaging detectors will be required for future grating spectrometers (Con-X), and probably also for wide-field imaging (XEUS, Gen-X)

- Technologies being explored to provide improvements
  - Better low-energy response
  - Better radiation tolerance
  - Better time resolution/faster readout rates

Future X-ray Imaging Detectors: Faster is Better

- Current CCDs have frame readout times of order seconds/frame.
- Faster readout (msec or less) offers many advantages:
  - * Reduced photon pileup
  - * Less dark current per readout, so can operate at higher temperature
  - * Less optical contamination per readout, so thinner optical blocking filters (better low-energy efficiency)
  - * Possibly better background rejection through temporal anticoincidence:
  - cf 99.9% rejection for ROSAT gas counter vs 99% for CXO/XMM CCDs
- Highly parallel readout (e.g., active pixel sensors like those in mobile phones!) may yield orders of magnitude increase in frame readout rate & integrated signal processing.

Comparison of X-ray and Optical
CCD Applications

Similarities

- Low noise is desirable (2-4 electrons RMS routine)

- Pixel size and area requirements are comparable

- Gate structure limits useful spectral range, so backside illumination is desirable

Differences

- X-ray devices must readout faster (~few s/frame) to count photons; requires framestore

- X-ray devices must have larger depletion depths (30-50 μm) for good QE and particle rejection; this requires higher resistivity (purer) silicon (by factor of ~10^3)

- X-ray devices must have extremely high charge transfer efficiency (CTI = (1-CTE) < 10^{-5}) at very low signal

- X-ray signal is very high contrast, so cross-talk rejection requirements may be more stringent

- X-ray devices have significant out-of-band sensitivity (e.g., UV, optical) that must be controlled

- Optical applications are more sensitive to pixel-to-pixel quantum efficiency variations (relatively high sky background), and optical response may be more sensitive to gate structure thickness variations

- Optical devices require relatively large full well capacity (by factor of 10-100) and larger dynamic range (16 bits vs 12 bits)