The effects of charge diffusion on soft X-ray response for future high-resolution imagers

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**Motivation**
Future solid state imagers for high-spatial-resolution X-ray missions such as AXIS and Lynx will require an unprecedented design of "tall and skinny" pixels: small pixels to sample the sharp PSF, and deep depletion for hard X-ray sensitivity. This presents challenges for the detection of soft X-rays, since the charge cloud produced by a photon near the entrance window diffuses to multiple pixels by the time it is collected at the rear surface, complicating energy reconstruction. We present simulations of this process to inform the design of such future detectors.

**Charge Diffusion Simulations**
We simulated the diffusion of charge clouds with Poisson_CCD (Lage+2017), a semiconductor simulator that models the electric field in the detector and solves Poisson's equation for the motion of charge carriers in that field. We ran this for a variety of notional back-illuminated (BI) CCDs with depletion depth of 50–100 μm. The cloud diffusion is well-modeled by a two-dimensional Gaussian for interactions throughout the device. For each notional detector and for a grid of photon energies, we simulated 50,000 photons attenuated by the Si and the resultant charge diffusion. Each charge cloud was randomly projected onto a grid of pixels as if it were read out, using different pixel sizes and adding Fano noise and various amounts of readout noise. The resultant "events" were processed similarly to X-ray data.

**Response vs. Pixel Size**
Below we show the response to monochromatic photons due to charge diffusion for various pixel sizes and high (top) and low (bottom) readout noise. Wider and shorter pixels provide better knowledge of the photon energy, especially at softer energy and with higher readout noise, where charge is lost below the threshold in neighbor "split" pixels.

**Response vs. Readout Noise**
Below we show the mean energy shift, QE, and response FWHM as a function of energy for two likely pixel sizes and various readout noise. Larger pixels yield substantial improvement in all metrics, but clearly reducing the readout noise is the most important factor for good response at low energies.

The rise in gain and drop in FWHM at low energies is an artifact of fitting a single Gaussian to multimodal histograms.

**Comparison to Real Data**
To validate the simulations, we simulated charge diffusion in a real X-ray detector for which we have substantial data, the MIT/Lincoln Laboratory CCID-41 BI device flown on Suzaku (Koyama+2007). We compared the simulations to data from X-ray-bright celestial sources and from ground calibration. The real data contain more multi-pixel events than the simulations predict, implying more charge diffusion in the real CCD. This could arise from incorrect modeling of diffusion at the backside interface or at the gate structure.

**Summary**
The simulations show that while larger pixels and thinner depletion improve the soft X-ray performance, reducing the readout noise has a dominant effect in all cases. Since compelling science requirements often compete technically with each other (high resolution, soft X-ray response, hard X-ray response), these results can be used to find the proper balance for a future high-resolution X-ray instrument.

**Future Work**
We will validate the simulations using ground data from newer CCID-80 devices, and explore sub-pixel positioning for various pixel sizes.

**References**
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Lage+2017, Jinst, 12, C03091
Koyama+2007, PASJ, 59, 23
Mushotzky+2018, SPIE, 10699-80

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