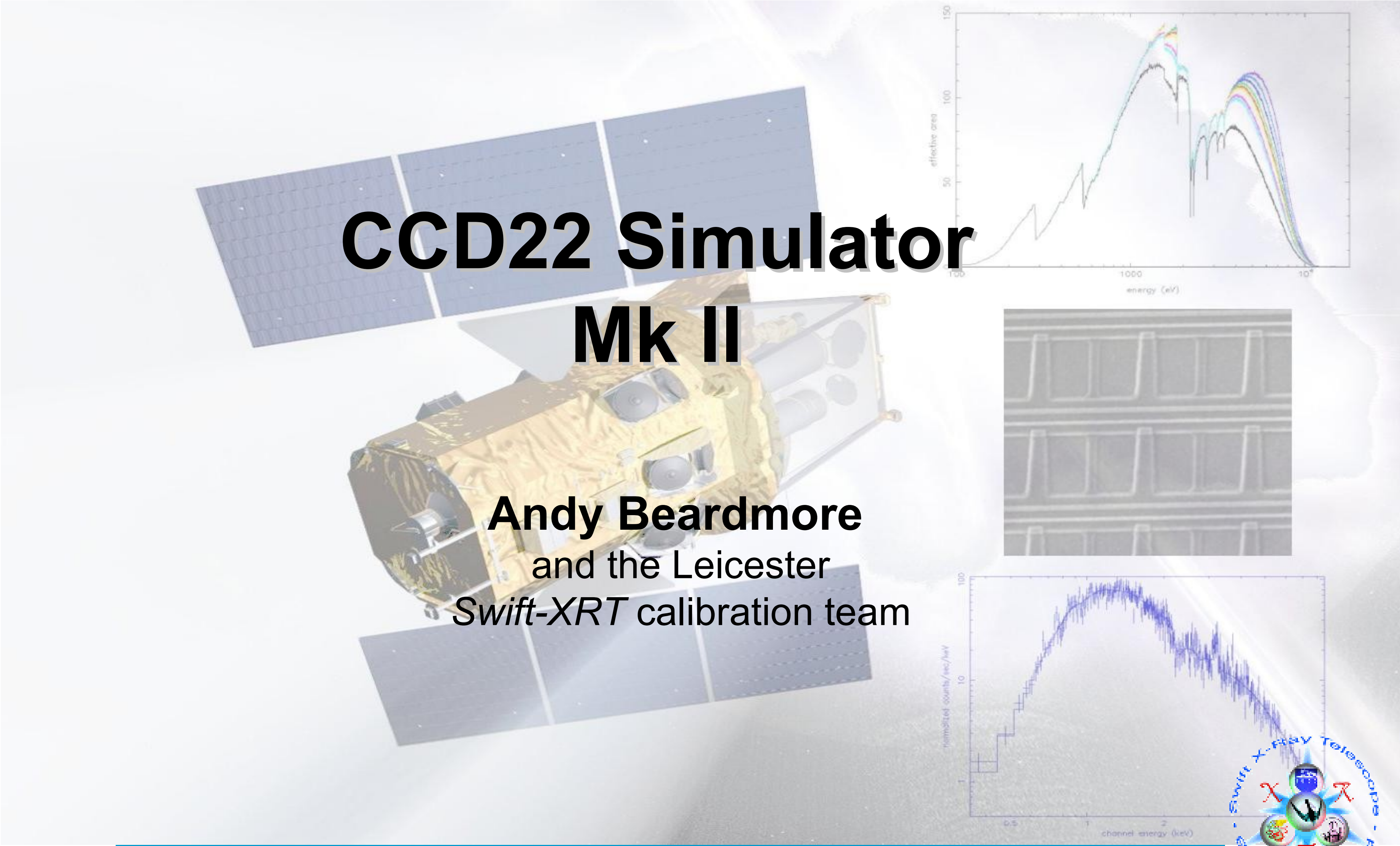


CCD22 Simulator
Mk II

Andy Beardmore
and the Leicester
Swift-XRT calibration team

Why Rewrite ?

- Existing code is written in FORTRAN-77(!)
- Only approximates the XRT onboard and ground s/w event recognition schemes
  - split event threshold is constrained to be same as event threshold
  - Grading schemes not identical

- Code base diverged between PC and WT
  - WT uses gaussian approx to line spreading
  - PC uses more rigorous “charge cloud spreading” model in field-free region
  - Hard-coded energy dependent shelf and line profile “fixes”
    - Ended up with two different WT codes with different shelf “fixes” for grade 0-2 and 0
- Most importantly - need to fix WT mode
  - Grade 1,2 redistribution clearly inaccurately
    - 10 row binning an afterthought

CCD22 Simulator MkII

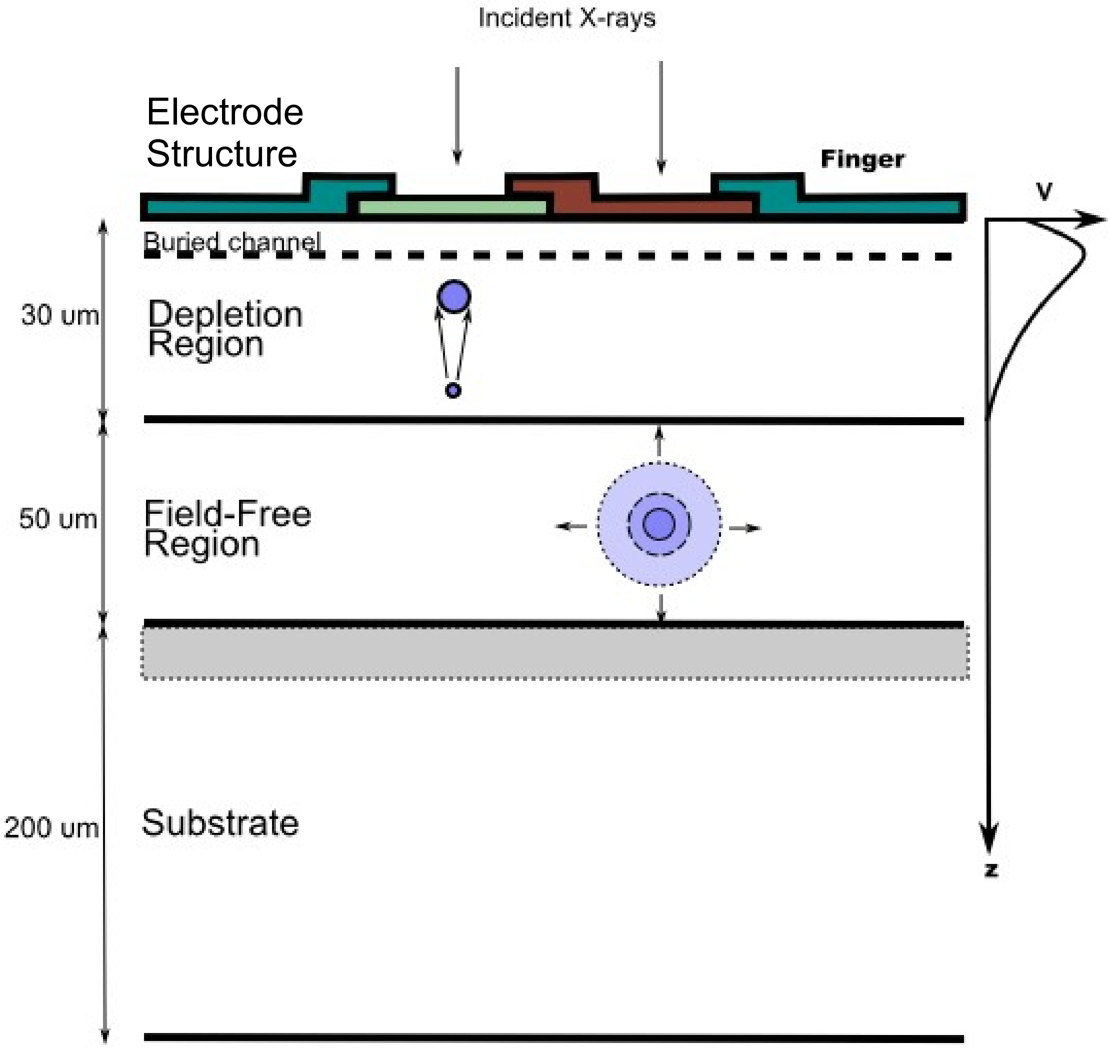
- Written in C++ with the aim to be modular.
- ReadoutMode base class
  - implements the image, store, and serial-register arrays; pixel charge accumulation
- WTRawFrame, PCRawFrame derived classes implement the specific readout modes, CTE and readnoise application
  - Image → Store transfer for PC
  - 10 row binning → serial register for WT
- WTMode, PCMode are further derived classes implement the event recognition and grading

- Generic source input. Photon obtained from
  - Photon/s/bin spectrum at top of CCD
  - Spatial distribution
    - Uniform source (circle or rectangle)
    - Drawn from the XRT PSF
- Full charge-cloud spreading
- Si-Kα flourescence
- Outputs an “event list” (bin, rawx, rawy, pha, grade)
- OpenMP parallelisation over the photon loop
  - 1 Million photon PC mode door source simulation takes 10 minutes using 10 cores.
  - Not so effective for WT mode

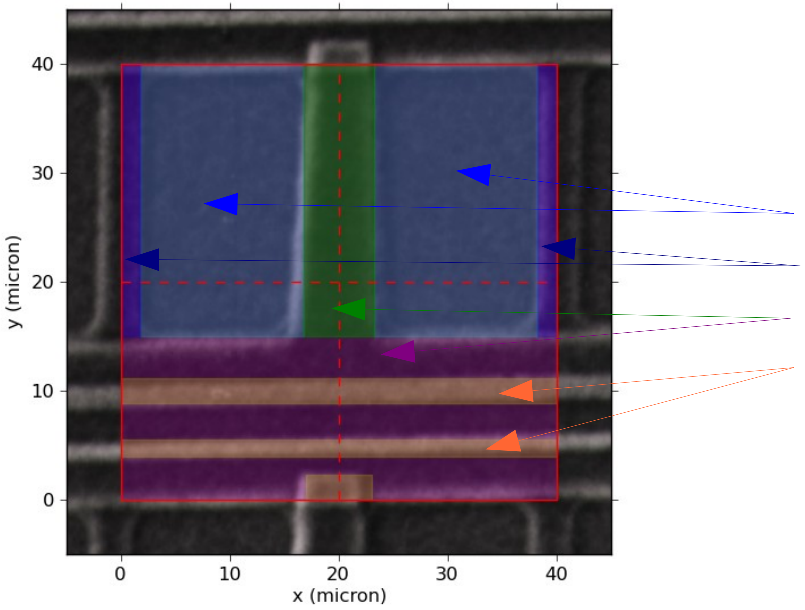
The difficult stuff – i.e. Physics!

- X-ray detection is determined by a photon's ability to pass through the electrode structure, while interacting in the active layer of the device
  - accurate Si, SiO2, Si3N4 absorption coefficients required → using ACIS values.
- Charge cloud spreading, followed by the pixel-mapping, event-recognition and grading determine how well the original photon energy can be recovered

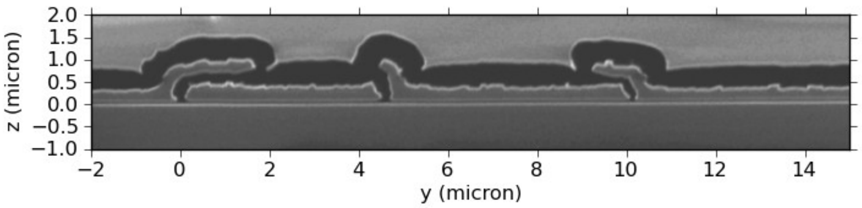
CCD Operation Overview



Open Electrode Structure



$$
\begin{aligned}
T_1 &= \exp(-0.1\,\mu_{SiO_2}) \\
T_2 &= T_1 \exp(-0.1\,\mu_{Si_3N_4}) \exp(-0.4\,\mu_{SiO_2}) \\
T_3 &= T_2 \exp(-0.25\,\mu_{Si}) \exp(-0.3\,\mu_{SiO_2}) \\
T_4 &= T_3 \exp(-0.25\,\mu_{Si}) \exp(-0.4\,\mu_{SiO_2})
\end{aligned}
$$



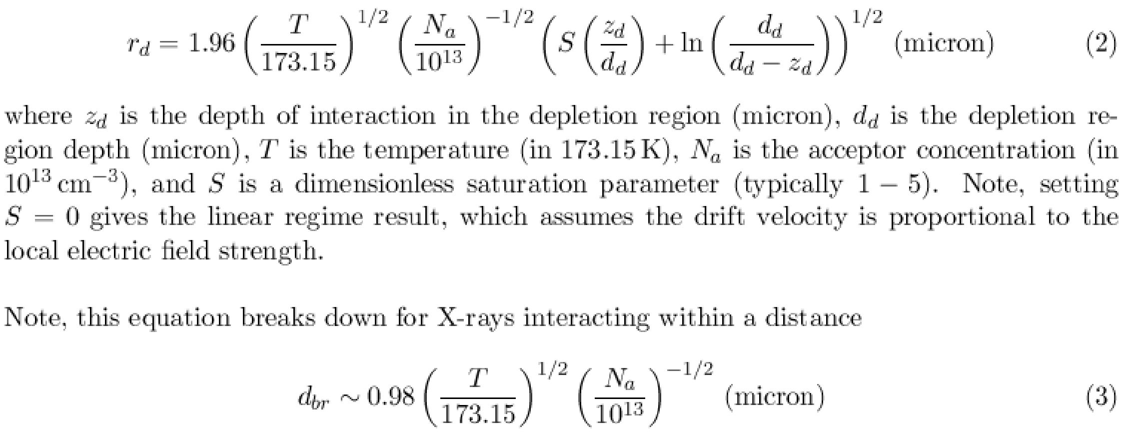
Charge cloud spreading

- Initial Size (Pavlov & Nousek 1999)
  - 3D Gaussian, with 2D cylindrical radius

$$r_i = 0.012E^{1.75}\,(\text{micron})$$

  - Less than 1 micron for energies of interest

- Depletion region (Hopkinson, 1984; PN 1999)
  - Expansion radius



$$r_d = 1.96\left(\frac{T}{173.15}\right)^{1/2}\left(\frac{N_a}{10^{13}}\right)^{-1/2}\left(S\left(\frac{z_d}{d_d}\right)+\ln\left(\frac{d_d}{d_d-z_d}\right)\right)^{1/2}\,(\text{micron}) \qquad (2)$$

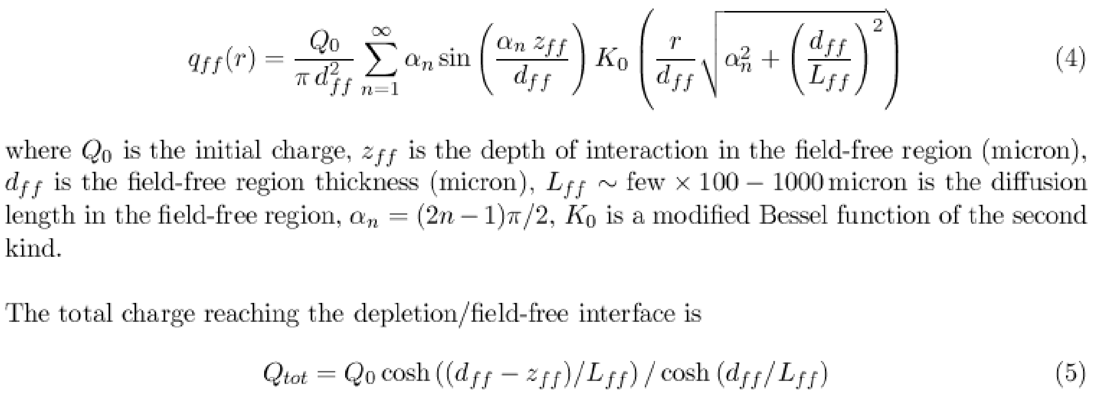
where z_d is the depth of interaction in the depletion region (micron), d_d is the depletion region depth (micron), T is the temperature (in 173.15 K), N_a is the acceptor concentration (in $10^{13}\,\text{cm}^{-3}$), and S is a dimensionless saturation parameter (typically $1-5$). Note, setting $S=0$ gives the linear regime result, which assumes the drift velocity is proportional to the local electric field strength.

Note, this equation breaks down for X-rays interacting within a distance

$$d_{br} \sim 0.98\left(\frac{T}{173.15}\right)^{1/2}\left(\frac{N_a}{10^{13}}\right)^{-1/2}\,(\text{micron}) \qquad (3)$$

Charge cloud spreading (ii)

- Field-Free region (Hopkinson, 1984; PN 1999)
  - Radial charge distribution at depletion/FF boundary



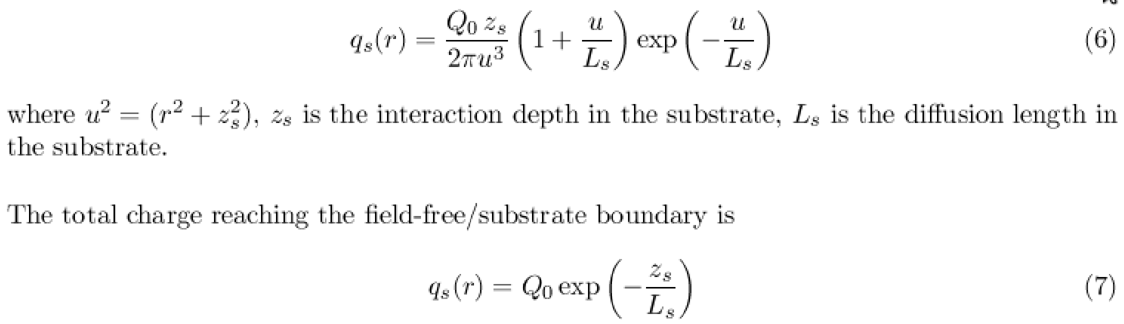
$$q_{ff}(r) = \frac{Q_0}{\pi\, d_{ff}^2} \sum_{n=1}^{\infty} \alpha_n \sin\left(\frac{\alpha_n\, z_{ff}}{d_{ff}}\right) K_0\left(\frac{r}{d_{ff}}\sqrt{\alpha_n^2 + \left(\frac{d_{ff}}{L_{ff}}\right)^2}\right) \qquad (4)$$

where Q_0 is the initial charge, z_{ff} is the depth of interaction in the field-free region (micron), d_{ff} is the field-free region thickness (micron), $L_{ff} \sim$ few $\times\, 100 - 1000\,$micron is the diffusion length in the field-free region, $\alpha_n = (2n-1)\pi/2$, K_0 is a modified Bessel function of the second kind.

The total charge reaching the depletion/field-free interface is

$$Q_{tot} = Q_0 \cosh\left((d_{ff} - z_{ff})/L_{ff}\right) / \cosh\left(d_{ff}/L_{ff}\right) \qquad (5)$$

- Substrate (Hopkinson 1984)
  - Radial charge distribution at substrate/FF boundary



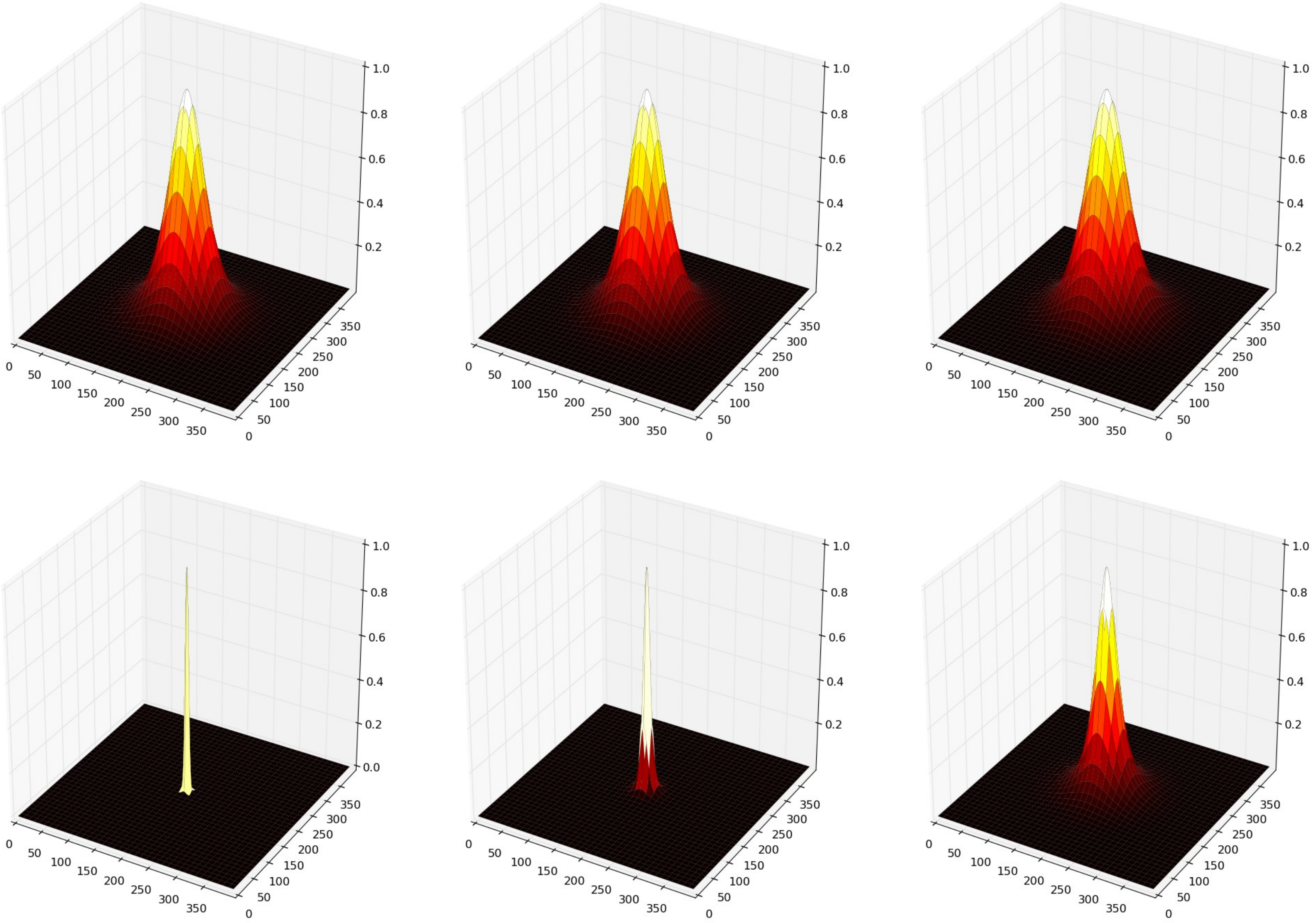
$$q_s(r) = \frac{Q_0\, z_s}{2\pi u^3}\left(1 + \frac{u}{L_s}\right) \exp\left(-\frac{u}{L_s}\right) \qquad (6)$$

where $u^2 = (r^2 + z_s^2)$, z_s is the interaction depth in the substrate, L_s is the diffusion length in the substrate.

The total charge reaching the field-free/substrate boundary is

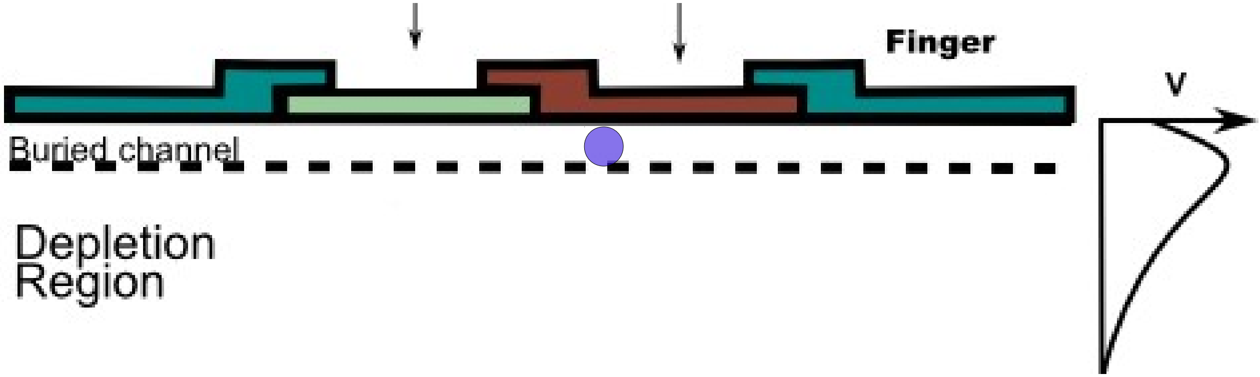
$$q_s(r) = Q_0 \exp\left(-\frac{z_s}{L_s}\right) \qquad (7)$$

2D Charge Distribution



Surface Loss Function

- Loss to surface states occur for events detected at low z (< buried channel depth of a few microns)

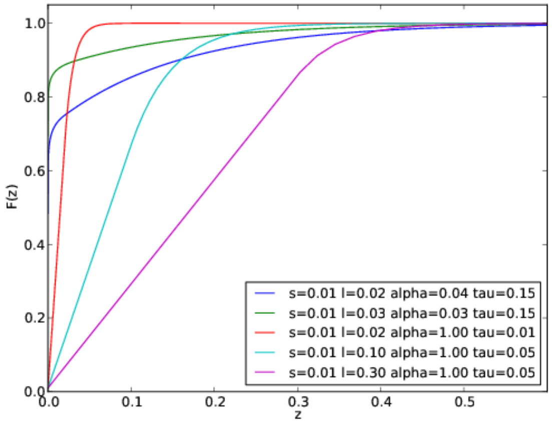


- Model with a loss function,

  $Q_o = Q_i \times f(z)$

where

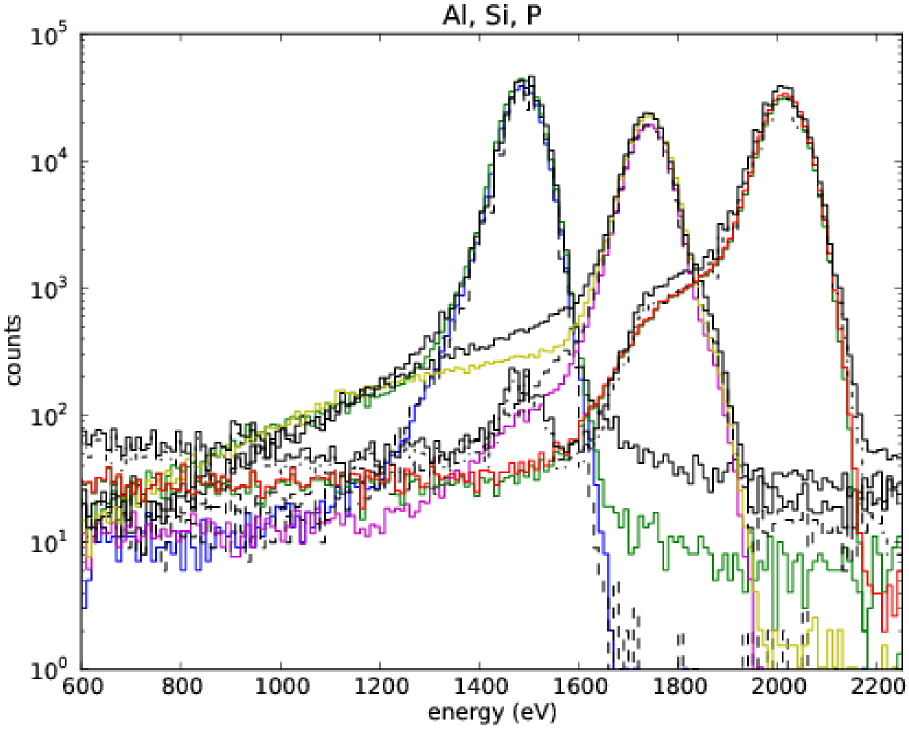
$$f(x) = S + B\,(z/l)^c \qquad (z<l)$$
$$= 1.0 - A\exp(-(z-l)/tau)$$



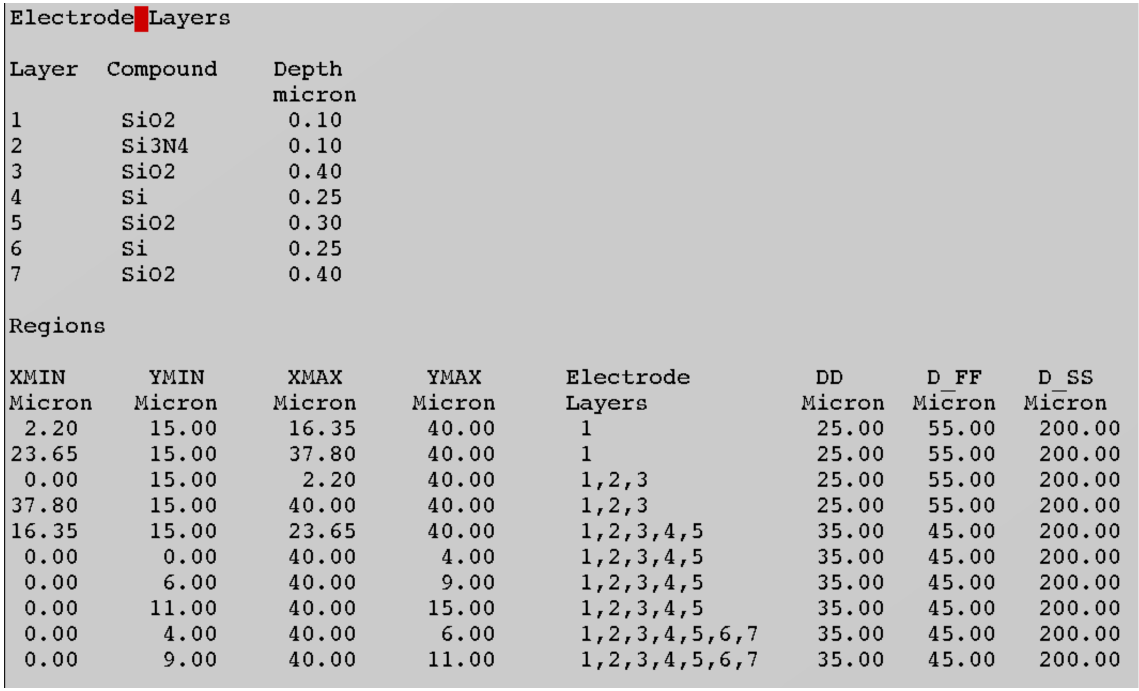
- Allow a different loss function for the closed and open parts of the electrode

Loss function (cont'd)

- Loss function is energy dependent and calibrated using pre-launch lab. data and Fe-55 door source data (obtained during LEO)
- linear absorption coeff varies greatly around the Si edge, as revealed by Al, Si & P Kα lines



- Operation controlled by an input file
  - Sets input source (spectrum, spatial model), pixel geometry, mode, thresholds, CTI, read noise, charge spreading params, etc
- Pixel geometry file



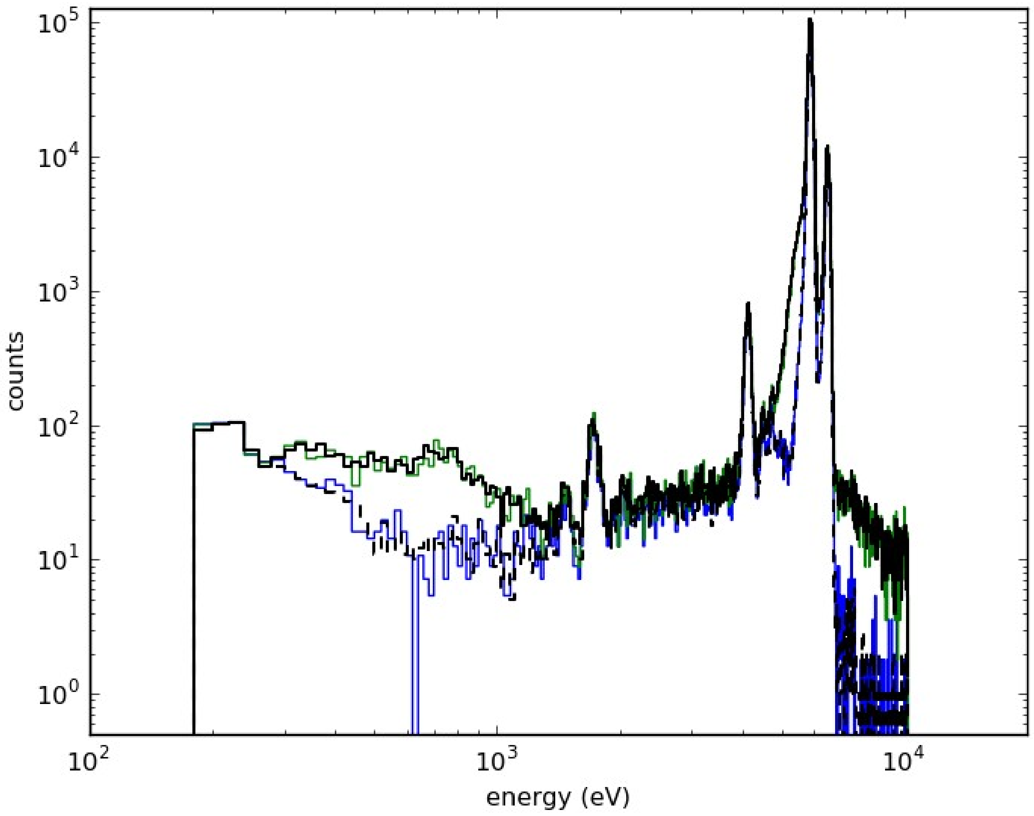
```
Electrode Layers

Layer  Compound    Depth
                   micron
1       SiO2        0.10
2       Si3N4       0.10
3       SiO2        0.40
4       Si          0.25
5       SiO2        0.30
6       Si          0.25
7       SiO2        0.40

Regions

XMIN      YMIN      XMAX      YMAX      Electrode         DD      D_FF    D_SS
Micron   Micron    Micron    Micron     Layers           Micron  Micron  Micron
 2.20     15.00     16.35    40.00       1                25.00   55.00   200.00
23.65     15.00     37.80    40.00       1                25.00   55.00   200.00
 0.00     15.00      2.20    40.00       1,2,3            25.00   55.00   200.00
37.80     15.00     40.00    40.00       1,2,3            25.00   55.00   200.00
16.35     15.00     23.65    40.00       1,2,3,4,5        35.00   45.00   200.00
 0.00      0.00     40.00     4.00       1,2,3,4,5        35.00   45.00   200.00
 0.00      6.00     40.00     9.00       1,2,3,4,5        35.00   45.00   200.00
 0.00     11.00     40.00    15.00       1,2,3,4,5        35.00   45.00   200.00
 0.00      4.00     40.00     6.00       1,2,3,4,5,6,7    35.00   45.00   200.00
 0.00      9.00     40.00    11.00       1,2,3,4,5,6,7    35.00   45.00   200.00
```

The Importance of Getting Good Grades

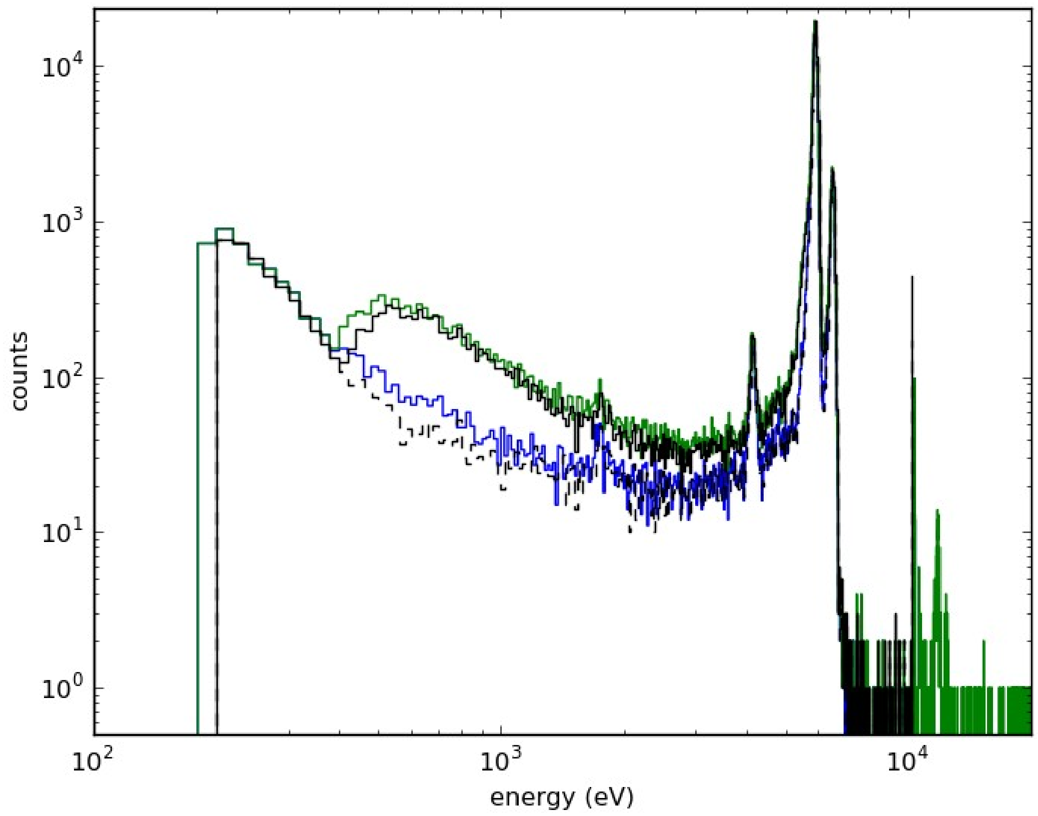


Final algorithm:

- Loop through each pixel (x, y)
- Test if PHA > thresh
- Test if pixel is the local max in 3x3
- Grade 3x3
- Leave 3x3 in image array
- Repeat over all pixels

The Importance of Getting Good Grades (ii)

WT mode test



Algorithm:

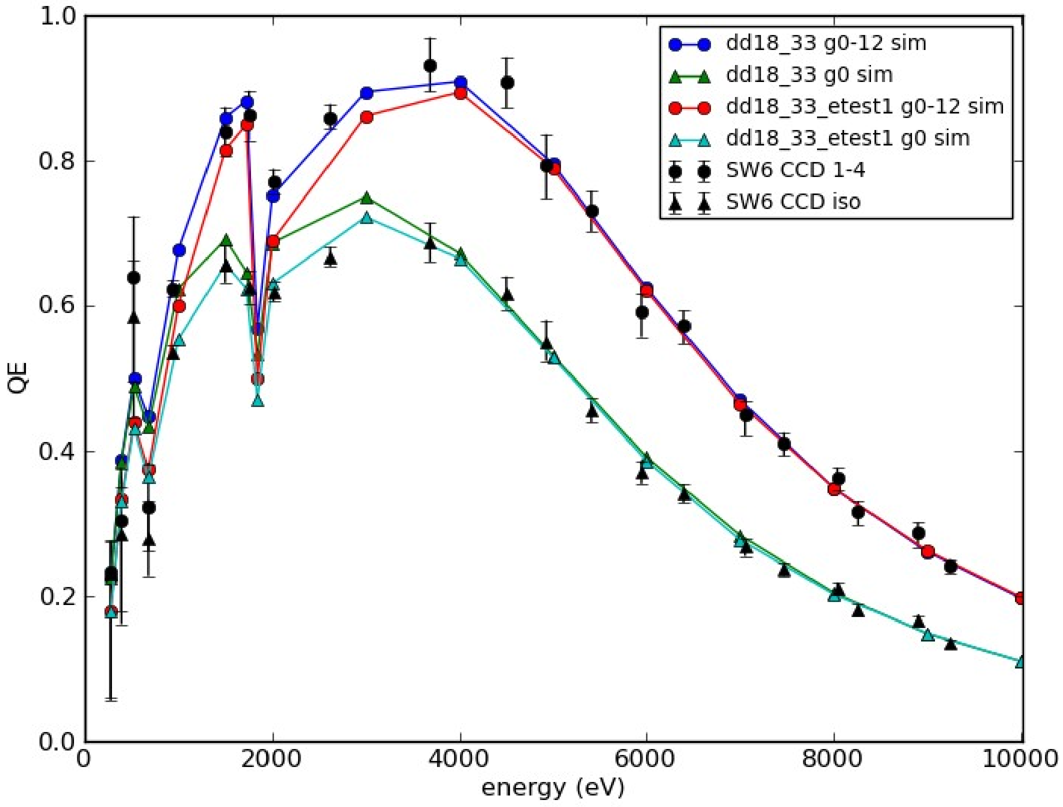
- Find next max PHA above threshold in 200 pixel readout array
- Extract 7 pixel array centred on the max PHA pixel
- Grade 7 pixel array, taking care with “don't care” pixels
- Mask out pixels in grade
- Repeat until no pixels remain above threshold

Simulation Results

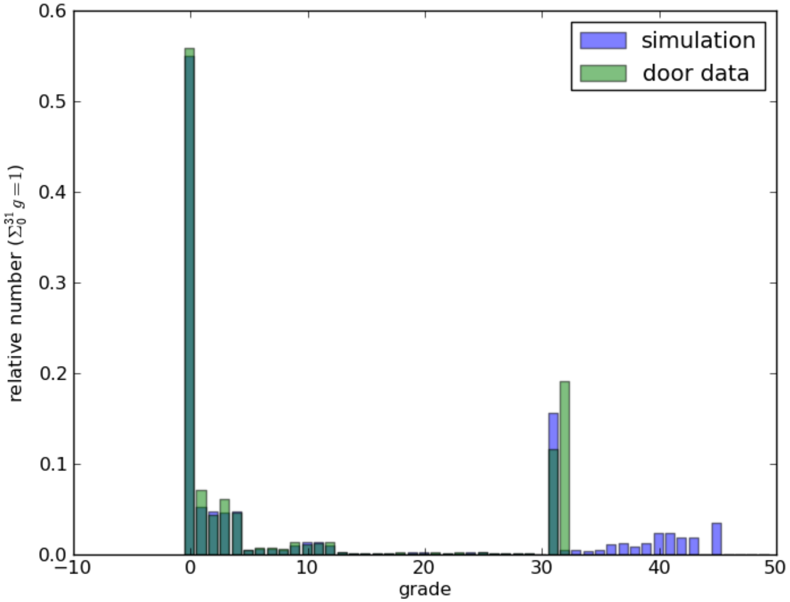
- Ideally the simulator output should match all three of the following :
  - QE
  - Grade ratios
  - Redistribution
- Found this a difficult goal to reach using the pre-established inputs (i.e. the electrode layer thicknesses, depletion layer thickness, field-free layer thickness)

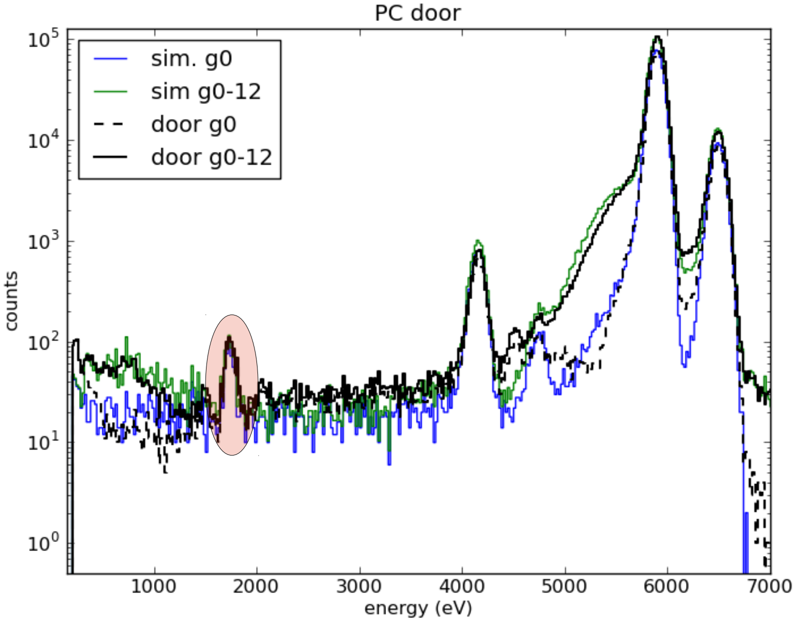
Results – PC QE

- QE comparison – lab data (Astrosat CCD, courtesy G. Hansford) & model



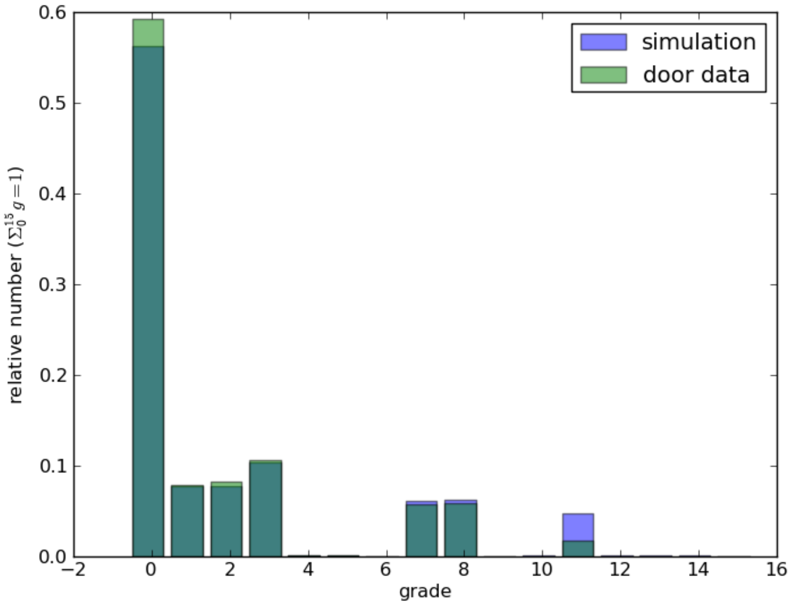
Results - PC

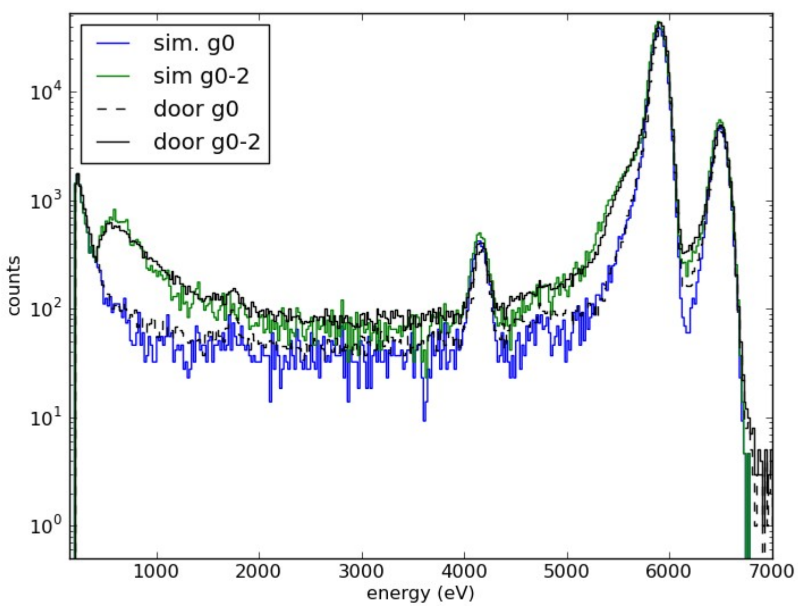




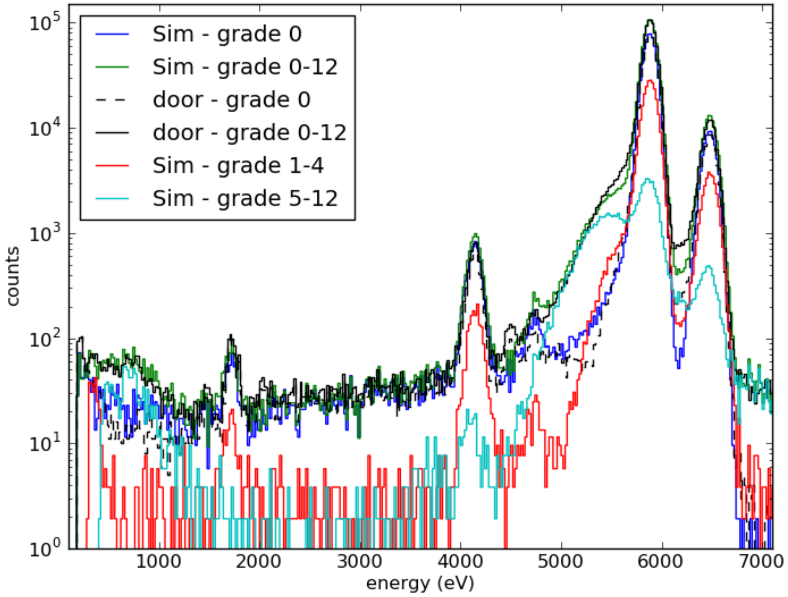
Si Kα mean free path X 1.7
to produce line flux

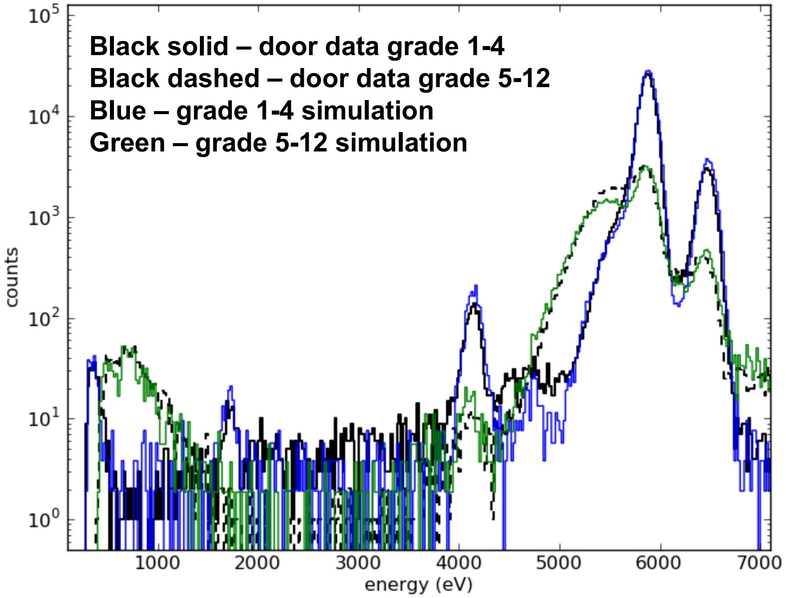
Results - WT


0.6
0.5
0.4
0.3
0.2
0.1
0.0
relative number ($\Sigma_0^{15} g = 1$)
−2
0
2
4
6
8
10
12
14
16
grade
simulation
door data


10^4
10^3
10^2
10^1
10^0
counts
1000
2000
3000
4000
5000
6000
7000
energy (eV)
sim. g0
sim g0-2
door g0
door g0-2

PC spectra – by grade

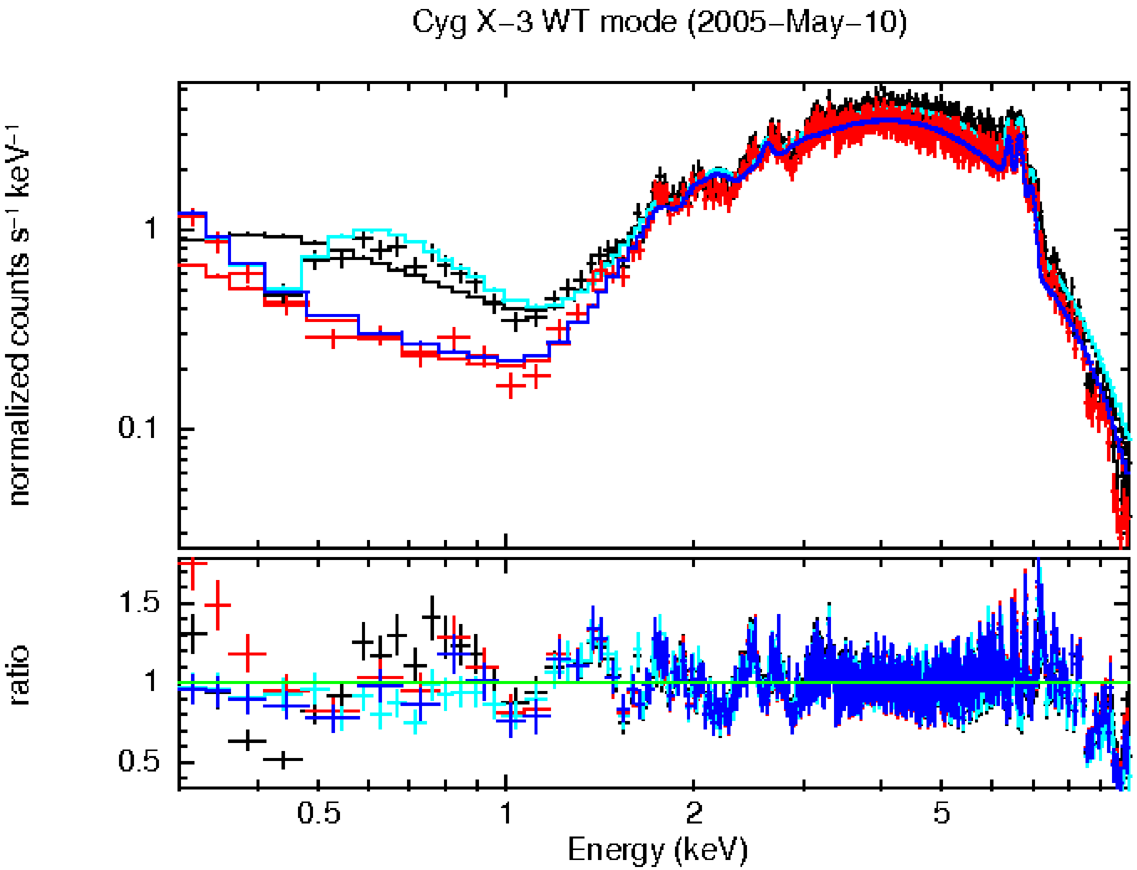




Black solid – door data grade 1-4
Black dashed – door data grade 5-12
Blue – grade 1-4 simulation
Green – grade 5-12 simulation

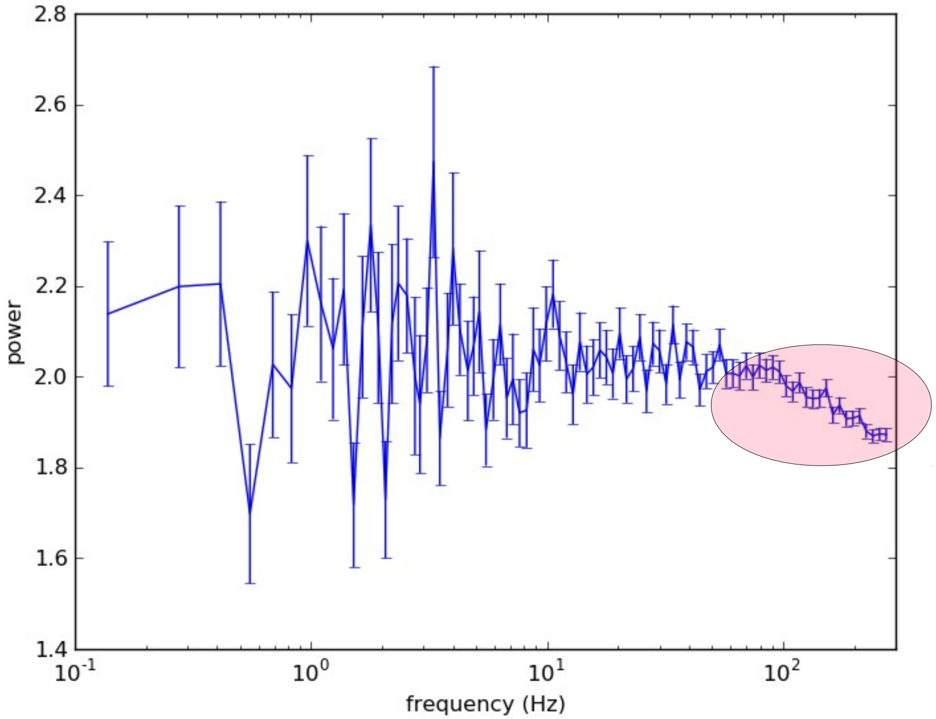
Test WT RMF

- Redistribution bump and low E turn up is more accurately modelled



WT simulation – power spectrum

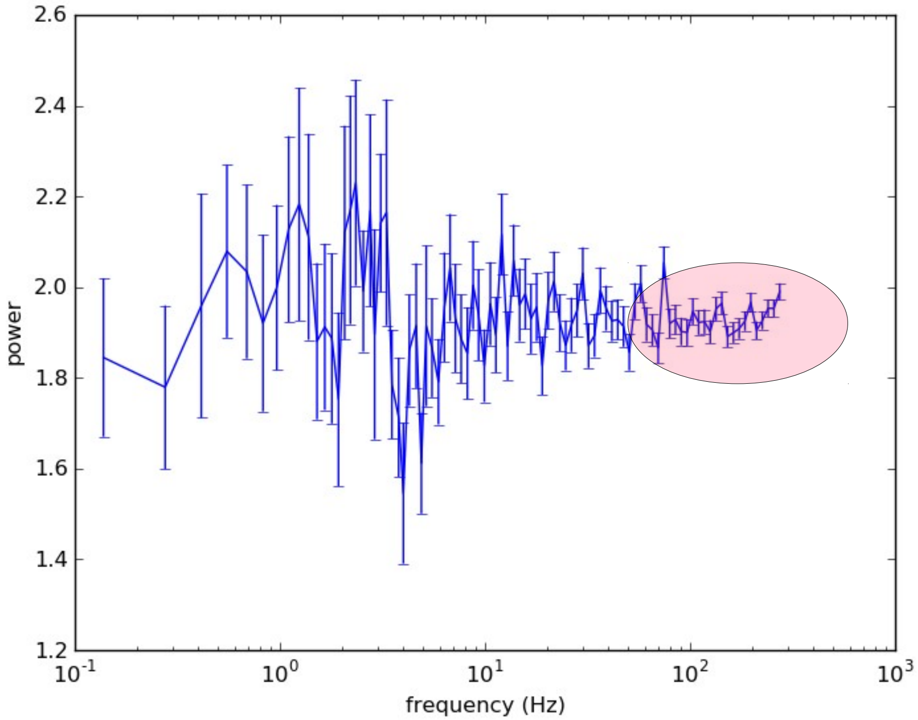
- Converted PSF Mn-Kα source event file to light curve and made a powerspectrum



- Fall-off in power at high frequencies, as seen in real WT data from hard sources
- Origin is event splitting at the 10 row boundary of multipixel events.

WT simulation – power spectrum (cont'd)

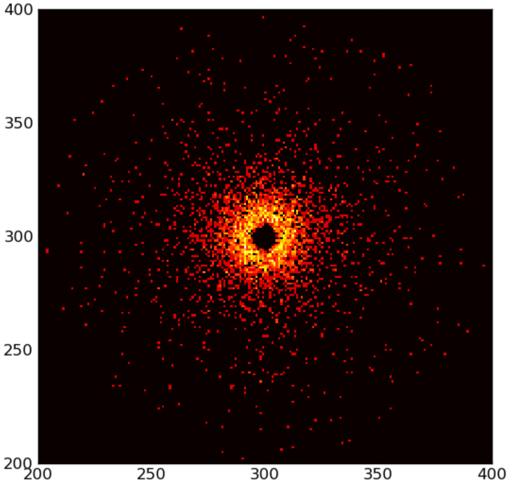
- Powerspectrum of a soft source (O-Kα line) simulation – i.e. nearly all single pixel events

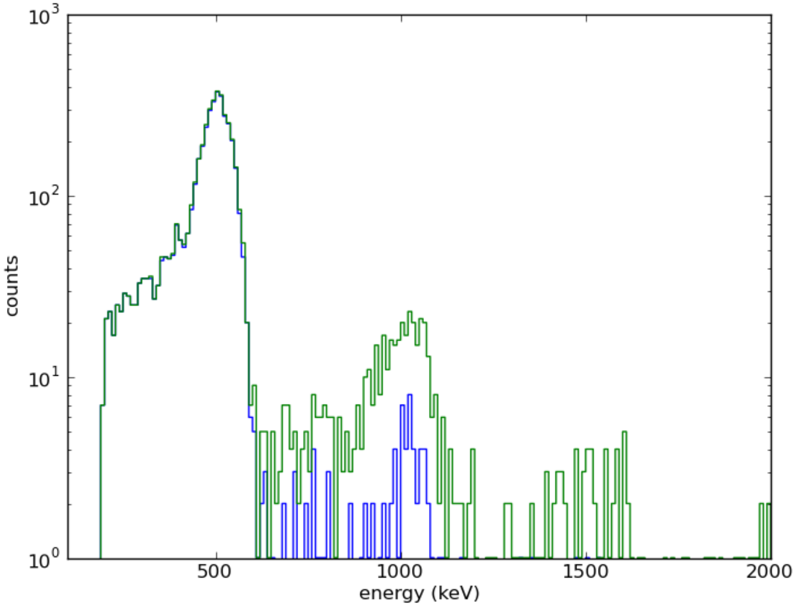


- No fall-off in power at high frequencies, as seen in real WT data from soft sources.

Pile-up

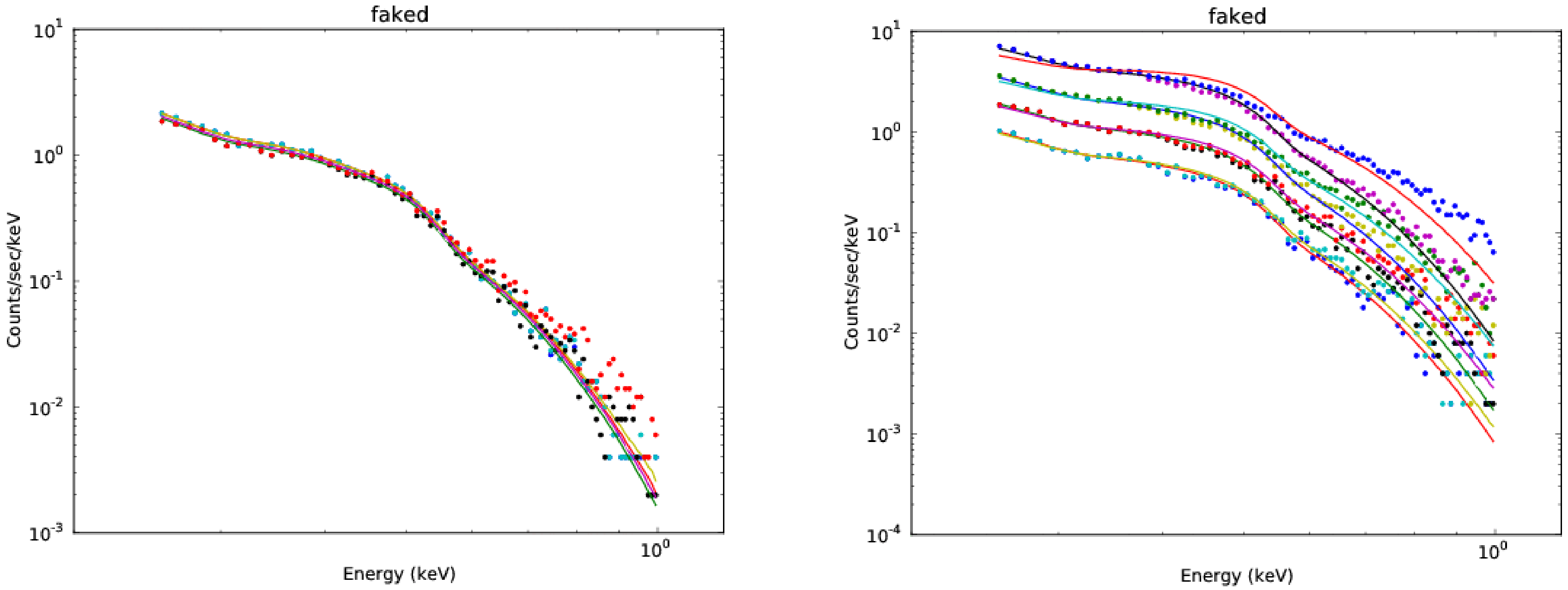
- Simulator naturally reproduces pile-up





Pile-up study

- Simulator naturally piles-up events



•WT simulation – default source input rate → CF=1.0

•PC simulation - default source input rate → CF=0.9

• Need to go to a rate of x0.1=0.03c/s to be free from pile up

ToDo

- Tweak the inputs to produce the best match of QE, grade fractions, redistribution
- Produce RMFs
  - Will have to match the temporal evolution of the spectral resolution for both modes and WT redistribution bump, plus change in in QE when the substrate voltage was altered
- Perform a detail study of the pile-up characteristics of our data