X-ray Analysis of Fully Depleted CCDs with Small Pixel Size

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Abstract

X-rays frames offer a lot of information about CCD. ^{55}Fe sources are traditionally being used for CCD gain and charge transfer efficiency (CTE) measurements. In addition X-rays can be used for the system linearity test. We demonstrate how spectral lines of ^{55}Fe and ^{241}Am rad. sources are used for system linearity measurements. The pixel size of modern scientific CCDs is getting smaller. The charge diffusion causes the charge spread among neighboring pixels especially in thick fully depleted sensors. This enables measurement of the charge diffusion using ^{55}Fe X-rays. On the other hand, the usual CTE characterization method based on single pixel X-ray events becomes statistically deficient. A new way of measuring CTE using shape and amplitude analysis of X-ray clusters is presented and discussed. This method requires high statistical samples. Advances in test automation and express analysis technique allows for acquiring such statistical samples in a short period of time. The lateral diffusion measured using e2v CCD250 is presented and implications for X-ray cluster size and expected cluster shape are discussed. The CTE analysis using total X-ray cluster amplitude is presented. This analysis can reveal CTE problems for certain conditions. The statistical analysis of average X-ray cluster shape is presented. The details of our measurement procedure are presented.

Keywords: CCD, charge diffusion, charge transfer efficiency, CCD X-ray detectors

1. INTRODUCTION

Specialized CCD sensors are being developed for the LSST camera. They are n-channel, fully depleted, back illuminated, $100\mu\text{m}$ thick devices with pixel size $10\mu\text{m}$. First prototypes have been produced and tested [1],[2].

The ^{55}Fe X-ray data are routinely collected as a part of our device characterization test suite [3]. The express analysis[3] of these data reports measured gain and noise values for all CCD channels. For example, the reported system noise in presented data was at the level of 6.5e-. Examples of express analysis output are shown below for the high statistics data set. ^{55}Fe run summary plots are shown in Fig.1. Black line

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Figure 1: X-ray spectra for each CCD segment. Segment count goes from left to right and top to bottom.

shows $K_{\alpha,\beta}$ fit. These plots are used for gain estimation. The ^{55}Fe X-ray spectral features: $\text{Mn } K_{\alpha,\beta}$ lines, escape peak and $\text{Si } K_{\alpha,\beta}$ peak can be used for system linearity test in low signal range, 470e- - 1760e-. The signal range for linearity test can be extended up to 16,000e- using ^{241}Am source producing dominating 59.54 keV line and a number of lower energy lines as well. The linearity tests are discussed in section 2 .

For many LSST tasks achieving a small PSF is critical. Thus LSST sensors are operated in over depletion mode. The bias voltage larger than needed for full depletion is applied to the device creating the electric field up to 6 kV/cm . In thick fully depleted CCDs, charge carrier transport from the back window to the gates is accompanied by charge diffusion. For details see, for example [4], [5] and measurement methods [6], [7], [8], [9], [10], [11]. We have developed a new method to obtain the characteristic diffusion σ value from analysis of the charge distribution in ^{55}Fe X-ray clusters [12], [13]. It is quite practical to use ^{55}Fe X-ray data for charge diffusion characterization as shown in section 3.

These data were obtained with CCD 250. The sensor was operated at -100°C in a cryostat equipped with a $10\mu\text{Ci}$ deployable internal ^{55}Fe source. Custom 4 channel preamplifiers were mounted on Dewar air side feed through. Data sets were acquired using Reflex controller. The readout speed was 545 kHz. The sensor with bad segments is deliberately chosen to demonstrate analysis sensitivity and power of ^{55}Fe method in uncovering sensor defects.

As seen in Fig.1 segments 10 and 11 demonstrate ^{55}Fe spectra degradation. Even though $K_{\alpha,\beta}$ peaks are visible the low energy tail washes out escape and Si peaks. The diagnostic of the cause is discussed in section 4. The use of X-rays for defect diagnostic and charge transfer efficiency (CTE) measurements as discussed in sections 4 and 5 correspondingly.

Table 1: ^{55}Fe spectra fit summary, using Fano factor 0.11 and pair creation energy 3.68 eV/pair.

Line	# X-ray $\times 10^3$	Peak position, adu	Peak width, σ , adu	Gain, e-/adu	Noise, e-
$Mn\ K_{\beta}$	138	455.26 ± 0.03	6.50 ± 0.02	3.874	6.99
$Mn\ K_{\alpha}$	1,001	413.98 ± 0.01	6.13 ± 0.01	3.870	6.55
<i>escape</i>	8.6	291.4 ± 0.3	6.07 ± 0.1	3.875	6.91
$Si\ K_{\alpha,\beta}$	4.8	122.7 ± 0.14	5.5 ± 0.1	3.875	6.68

2. System Linearity Measurement using Characteristics X-rays

The system response in the small signal range of thousand electrons or less is essential input for astrophysics analysis, particularly for analysis of faint objects. The system linearity in this range is difficult to measure using flat field image technique. The mechanical shutter limits the linearity accuracy for short exposures needed to cover the small signal range. On the other hand the rich structure of the ^{55}Fe spectra enables such measurements in the range 470 - 1760e-.

The ^{55}Fe atom decays through electron capture mechanism. In this process the ^{55}Mn atom is produced in excited state with a K-shell vacancy. The excitation energy is released by emitting either X-rays or Auger electrons. The most probable X-rays are K_{α} , with energy 5.895 keV and K_{β} , with energy 6.490 keV. They interact with Si and either produce a single cluster containing the full X-ray energy or $Si\ K_{\alpha,\beta}$ escapes from that cluster. In this case the energy left in the cluster is equal to $E(Mn\ K_{\alpha,\beta}) - E(Si\ K_{\alpha,\beta})$ and a separate $Si\ K_{\alpha,\beta}$ cluster can be formed. The transition probabilities, line energies and average energy required for pair creation in Si can be found, for example in [14]. The major peaks seen in Fig.1,2 correspond to (from left to right) $Si\ K_{\alpha,\beta}$, $Mn\ K_{\alpha}$ escape peak, $Mn\ K_{\alpha}$, $Mn\ K_{\beta}$. The energy of each line is known with very high precision.

Observed peak positions were obtained fitting the corresponding line with Gaussian+background model functions. Examples of the line fits are displayed in Fig.1,2,3. The MINUIT package [15] was used for fitting. To study the stability and robustness of the fits, model functions being varied from single Gaussian to 2 Gaussians+polynomial background. It was found that for all lines fits are pretty robust. It is attributed to the fact that peaks are well above the background. For example, the most complex background is under the $Mn\ K_{\alpha}$ peak but the background level is 600 times less than the peak height itself. So even simple Gaussian fit in the limited range is sufficiently accurate in this case. Obtained results are summarized in Table 1. Conversion gain values were calculated for X-ray lines as $gain = N(e-)/peak\ position(a.d.u.)$. The number of electrons for not resolved peaks is the weighted average of underlined lines. The average gain is 3.873e-/adu with deviations from the average less than 0.1% The system noise was obtained subtracting the natural line width from the measured line width. The system noise estimated this way is in agreement with noise reported by express analysis.

Figure 2: ^{55}Fe spectra for channel 2. Color lines show fit results: black - ^{55}Mn $K_{\alpha,\beta}$ lines; red - escape peak; green - Si $K_{\alpha,\beta}$ peak;

Figure 3: ^{241}Am spectra for channel 15. Color lines show fit results: black - 59.541keV line; green - ^{68}Er $K_{\beta 1,3}$ peak; red - ^{68}Er $K_{\alpha 1,2}$ lines; blue - ^{237}Np 26.345 keV line; yellow - ^{237}Np $L_{\beta 1}$ line plus unidentified peak; magenta - 8.14 and 9.02 keV unidentified peaks.

It is attractive to extend the signal range using higher energy X-rays. The ^{241}Am is one convenient source providing strong 59.5 keV line. These X-rays penetrate the Dewar window. In our case, 0.6" fused silica glass attenuate the X-ray flux by about factor 2. The Si is mostly transparent for these X-rays. The absorption length in Si for 59.5 keV X-ray is ~ 100 times longer compare to 5.9 keV. This means only $\sim 0.7\%$ of these X-rays interact in 100 μm thick CCD. So, ^{241}Am source activity should be accordingly higher to acquire high statistical data samples in a short period of time.

The ^{241}Am atom decays emitting alpha particle and producing the ^{237}Np atom in excited state (for reference see [16–18]). The excitation energy of ^{237}Np and emitted alpha particle energy are related. In $\sim 84\%$ ^{237}Np excitation is 59.541 keV. This excitation is released most often by emitting 59.541 keV X-ray with yield 0.36 X-rays per alpha particle. From 59.541 keV level the transition can also go through 33.196 keV level with emission of 26.345 keV X-ray. The relative probability of this transition is $\sim 7\%$. The subsequent cascade of transitions generates lower energy L X-rays and 17.751 keV $L_{\beta 1}$ and 13.946 keV $L_{\alpha 1}$ lines are the strongest. The acquired ^{241}Am spectra for channel 15 is shown in Fig.3. The expected ^{237}Np lines: 59.541 keV, 26.345 keV and 17.751 keV are identifiable in the spectra. The Fig.3 spectra shows that ^{93}Np L lines are greatly attenuated by the Dewar window. To enable the use of these lines for calibration the source should be placed inside the Dewar.

Unexpectedly, strong lines at 49.128 keV and 48.221 keV appear in the spectra. These are ^{68}Er $K_{\alpha 1}$ and ^{68}Er $K_{\alpha 2}$ lines, marked by the red curve on the Fig.3 plot. The ^{68}Er K_{β} lines are also present. The

Table 2: Linearity summary

Line	Energy, keV	Peak position, adu	Scale factor, eV/adu	# X-rays $\times 10^3$
<i>Mn K$_{\alpha}$</i>	5.895	417.49 ± 0.02	14.12	269
<i>Mn K$_{\beta}$</i>	6.490	459.39 ± 0.07	14.13	36
<i>Er K$_{\alpha 2}$</i>	48.221	3422.8 ± 0.2	14.09	59
<i>Er K$_{\alpha 1}$</i>	49.128	3487.5 ± 0.2	14.09	100
<i>Er K$_{\beta}$</i>	55.617	3945.4 ± 0.6	14.10	22
<i>Np</i>	59.541	4226.83 ± 0.07	14.09	440

$^{68}\text{Er } K_{\beta 1}$ and $^{68}\text{Er } K_{\beta 3}$ lines, 55.681 keV and 55.494 keV correspondingly, can not be resolved because their natural line width is larger than their separation. The $^{68}\text{Er } K_{\beta 2}$ line, 57.21 keV is visible. This line has not been fitted because of the relatively small signal to background ratio.

Initially the presence of ^{68}Er was a puzzle and possible contamination of both radioactive source and the Dewar window was checked using a HPGe detector. The result was negative, no contamination was found. Then the material analysis of AlN ceramic substrate was performed by John Warren. This analysis revealed the presence of ^{68}Er in ceramic. ^{68}Er atoms were excited by 59.541 keV X-rays and CCD detected their fluorescence. These lines can be used for calibration purposes. It should be noted that fluorescence excited by ^{241}Am 59.5 keV X-rays can come from variety of materials. Only strong, easily identifiable fluorescence lines were used in this analysis.

Two data sets, ^{55}Fe and ^{241}Am were taken sequentially. The results are summarized in Table 2. The systematic error in the fitted peak position is estimated to be $\sim 0.1\%$. The device is found to be quite linear. The maximum deviation from the average conversion factor is 0.2% in the range from 5.9 keV to 59.5 keV, 1600e- to 16000e- correspondingly.

3. Charge Diffusion. Measurement Method and Results

The initial charge cloud size generated by ^{55}MnK X-rays is very small. Initial size can be estimated from the electron range in silicon $0.012 \cdot E_{\gamma}^{1.75}$ [19], where E_{γ} is the X-ray energy in keV and range is in μm . For 5.9keV X-rays the range is $\sim 0.27\mu\text{m}$. The range is much larger, $\sim 30\mu\text{m}$ for 59.5keV electrons. Thus higher energy X-rays are not suitable for diffusion studies and only ^{55}Fe data were used for this analysis. During the transport from the point of generation to the gates charge cloud diffuses. The shape of diffused cloud is essentially Gaussian[4],[5]. The charge sharing between neighboring pixels depends on the charge cloud size at the gates and the position of the conversion point in the pixel. The 2D Gaussian charge distribution can be described by 4 parameters: conversion point coordinates, σ , and total amplitude. These parameters

can be determined for an individual X-ray if the cluster contains at least 4 pixels with amplitudes above the noise (with fewer pixels only an upper estimate on the cluster width can be obtained). The accuracy of these estimates depends on the signal to noise ratio of the cluster pixels. The low CCD noise allows for measurement of small diffusion sigmas even though the pixel size is 2-3 times larger than σ . Details of this method are presented in [12],[13]. Here the focus is on results and their implications.

The diffusion analysis has been performed on high statistics data set. The read out noise in this set was $\approx 7e-$. The measured σ values for first 8 channels are shown in Fig.4. The sigma distributions peak at

Figure 4: Measured diffusion sigma values for 8 segments.

$3.6\mu m$ for all segments in a good agreement with early measurements. There are no segment to segment variations as expected.

The characteristic diffusion value knowledge can be used to derive general properties of X-ray clusters. Lets construct the average cluster assuming uniform distribution of X-rays along sub-pixel coordinates. This can be done analitically by convoluting 2D Gaussian cluster shape with uniform distribution in x- and y-coordinates. The average cluster shape and its variability are shown in Fig.5.

4. Defect diagnostics with X-rays

X-ray spectra show low energy tails in segments 10 and 11. More information is needed to understand the cause. Such information can be obtained from the same X-ray data set. The CTE plots for segment 11, as an example, shown in Fig.6. This figure shows that X-ray spectra are normal in some parts of this segment and are degraded in others. It is possible to pinpoint bad areas using features of the ^{55}Fe X-ray spectra itself. The largest amount of X-rays belong to K_{α} and K_{β} lines. The window framing these lines can be set and amount of events inside this window is counted depending on coordinates. The $K_{\alpha,\beta}$ count has been done in pads 20×11 pixels. In other words the segment area has been divided into 250 rectangular

Average Hit Profile

Pixel r.m.s.

Figure 5: Average K_α hit 2D profile and variability, r.m.s., in each pixel.

138 pads and $K_{\alpha,\beta}$ events have been counted in each pad. The Fig.7 shows $K_{\alpha,\beta}$ count for all segments. The
 139 areas where $K_{\alpha,\beta}$ events disappear are clearly seen in segment 10 and 11. Large number of traps was found
 140 in this areas using pocket pumping technique.

141 5. CTE measurements with X-rays

142 The diffusion spreads charges over multiple pixels and number of single pixel clusters is very limited. So,
 143 using single pixel clusters for CTE measurements is not practical. From average hit properties discussed
 144 in section 3 follows that more than 99.9% energy is contained in a 3×3 zone around pixel with maximum
 145 amplitude. This zone always contains at least 99.5% of X-ray energy. Using this zone to measure X-
 146 ray parameters is an example of aperture photometry application. Thus CTE measured using zone total
 147 amplitude is arguably a good quantity to describe the charge loss in CCD readout process. This technique
 148 has been applied to the high statistics data set. Plots illustrating CTE analysis are shown in Fig.8 for
 149 segment 2 in normal operational conditions, $T = -100^0C$. In these conditions CTE is better than 0.999999

Figure 6: CTE plots for segment 11 at normal operating conditions.

in both serial and parallel directions. By lowering CCD temperature one can induce CTE degradation. Plots obtained at $T = -150^{\circ}\text{C}$ are shown in Fig.9 for segment 2. The CTE measured in these conditions is 0.999928 in serial direction and still better than 0.999999 in parallel direction. This corresponds to a loss of $\approx 56e-$ after 500 serial transfers and corresponding charge transfer inefficiency, CTI is $7.2 \cdot 10^{-5}$.

6. Average X-rays cluster shape and its use for CTE.

There is a worry that aperture CTE overestimate the CTE value. The central pixel, for example, might actually loose more charge then estimated using aperture CTE value. To check this we use the average pixel profile constructed both for small and large number of transfers. The construction of the profile introduced variability of the signal in the profile bins as seen in Fig.5. A large number of clusters is needed in order to achieve sufficient precision in the average pixel profile. For example, to reach 1e- r.m.s. accuracy about 30,000 clusters are needed. There are hundreds thousands X-rays in our high statistical sample and sub electron accuracy can be reached. The average K_{α} clusters were constructed for data sets taken at -100°C and -150°C . The number of clusters used for any segment zone was more than 200,000. Thus our accuracy level is $\approx 0.4e-$. The average clusters for normal conditions are symmetrical. The differences left-right, top-bottom are all within a few sigmas. The average clusters for segment 2 at -150°C are shown in Table.3 and Table.4. The segment was divided into two halves in serial direction. Table.3 shows average cluster in the first half with number of transfers from 0 to 250 and 125 transfers on average. Table.4 shows cluster in the second half with number of transfers from 250 to 500 and 375 transfers on average. The right-left

Figure 7: $K_{\alpha,\beta}$ count for all segments.

difference in the central row is $5.4e-$ in Table.3. The same difference in Table.4 is $16.4e-$. Considering the average number of transfers, 125 in the first case and 375 in the second, the excess of charges in the tail per transfer is essentially the same. Using the number of electrons in the central pixel one can calculate CTE in extended pixel response, EPER, style. This calculation gives CTE value 0.999950 and CTI is $5.0 \cdot 10^{-5}$ correspondingly. EPER method is sensitive to short release times ("fast" traps) and aperture method is sensitive to long release times ("slow" traps). Average cluster analysis gives insight into both time domains. The aperture method could be refined by addition of the charge redistribution analysis within the aperture.

CONCLUSIONS

It is demonstrated that X-rays analysis is a powerful tool for CCD characterization. X-rays can be used to measure system gain and linearity; characterize sensor PSF; reveal and pinpoint defect sites; measure

Figure 8: CTE plots for segment 2 at $T = -100^{\circ}C$.

CTE. X-ray sources provide characteristic X-rays with well known energy. These characteristic lines can be used for absolute calibration of the system linearity in the range from $470e^{-}$ to $16000e^{-}$. The usefulness of ^{55}Fe and ^{241}Am sources was demonstrated. Further improvements can be achieved placing both rad. sources inside the Dewar and adding more sources, for example ^{133}Ba . This will enable to use ^{237}Np 13 - 18 keV L-lines and Cs 30 keV K-lines and 4.5 keV L-lines.

CCDs with small pixel sizes and low read-out noise were used for charge carriers diffusion measurement. These measurements were performed using e2v CCD 250 with pixel size $10\mu m$. In this case noise level required for reliable diffusion estimate should be below $\sim 10e^{-}$. The measured on LSST prototype CCDs characteristic diffusion sigma corresponds to blue PSF value $0.17''$ (FWHM) for LSST plate scale.

It is shown how X-ray analysis reveals and pinpoints defect sites. The CCD with defects presented in some sectors was chosen to demonstrate this technique.

The X-ray average cluster shape analysis was used for CTE measurements. This approach provides

Figure 9: CTE plots for segment 2 at $T = -150^{\circ}\text{C}$.

practical and robust measurements when high statistical samples are available.

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Table 3: Average cluster profile close to readout node.

y/x	0	1	2
0	25.4 ± 0.1	152.2 ± 0.4	29.7 ± 0.1
1	151.3 ± 0.4	879.9 ± 0.5	156.7 ± 0.4
2	25.6 ± 0.1	152.6 ± 0.5	29.7 ± 0.1
sum	202.3 ± 0.4	1184.7 ± 0.7	216.1 ± 0.4

Table 4: Average cluster profile away from readout node.

y/x	0	1	2
0	22.5 ± 0.1	146.9 ± 0.4	31.5 ± 0.1
1	144.6 ± 0.4	871.1 ± 0.5	161.0 ± 0.4
2	22.7 ± 0.1	147.2 ± 0.4	31.7 ± 0.1
sum	189.8 ± 0.4	1164.2 ± 0.7	224.2 ± 0.4

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