Modelling charge transfer in a radiation damaged Charge Coupled Device for Euclid

David J Hall*, Andrew Holland, Neil Murray, Jason Gow, Andrew Clarke
e2v Centre for Electronic Imaging, DPS, The Open University, Milton Keynes, MK7 6AA, UK

ABSTRACT

As electrons are transferred through a radiation damaged Charge Coupled Device (CCD), they may encounter traps in the silicon in which they will be captured and subsequently released. This capture and release of electrons can lead to a 'smearing' of the image. The dynamics of the trapping process can be described through the use of Shockley-Read-Hall theory, in which exponential time constants are used to determine the probability of capture and release. If subjected to a hostile radiation environment, such as in space where the dominant charged particle is the proton, these incident protons can cause displacement damage within the CCD and lead to the formation of stable trap sites. As the trap density increases, the trapping and release of signal electrons can have a major impact on the Charge Transfer Efficiency (CTE) to the detriment of device performance. As the science goals for missions become ever more demanding, such as those for the ESA Euclid and Gaia missions, the problem of radiation damage must be overcome. In order to gain a deeper understanding of the trapping process and the impact on device performance, a Monte Carlo simulation has been developed to model the transfer of charge in a radiation damaged CCD. This study investigates the various difficulties encountered when developing such a model: the incorporation of appropriate clocking mechanisms, the use of suitable trap parameters and their degeneracy, and the development of methods to model the charge storage geometry within a pixel through the use of three-dimensional Silvaco simulations.

Keywords: CCD, radiation damage, simulation, CTI, CTE, Euclid

1. INTRODUCTION

The effects of radiation-induced damage in a Charge Coupled Device (CCD) on the images produced have been studied in great depth for many space missions. As the requirements on the cameras used in orbit become ever-more demanding, the impact of the radiation-induced damage has greater implications on the ability to achieve the goals set. Whilst an understanding of the effects on the images produced is essential, one must consider possible ways to reduce the impact of the radiation damage through operational changes and through the use of post-processing techniques to remove the effects. An accurate simulation of charge transfer in a radiation-damaged CCD can be used to aid both methods, although several obstacles must first be overcome. In this paper, the approach to modelling charge transfer in CCDs in general is considered alongside the difficulties that may be encountered and therefore the specific details of the CCD itself are not included.

2. EUCLID AND WEAK LENSING

The ESA Euclid mission aims to investigate how the Universe originated and from what it is made [1]. One of the primary goals is to understand the nature of dark matter and dark energy through the accurate measurement of the expansion of the Universe [2]. The mission will target galaxies (and clusters of galaxies) out to z~2, covering 15000 deg^2 in a wide extragalactic survey.

One method to investigate the nature of dark matter and dark energy is through the study of Weak Gravitational Lensing (WGL). The effects of WGL can be seen through the elliptical distortion of an image. Figure 1 shows the effect of different strengths of lensing on a circularly symmetrical image alongside an example of lensing from galaxy cluster Abell 1689. In order to measure extent of the WGL, one must therefore measure the change in ellipticity in the image. Unfortunately, WGL is not the only factor that can affect the measured ellipticity and one must consider the effects of radiation damage on the CCD used to create the image.

*d.j.hall@open.ac.uk; phone +44 (0)1908 659 579; www.open.ac.uk/cei

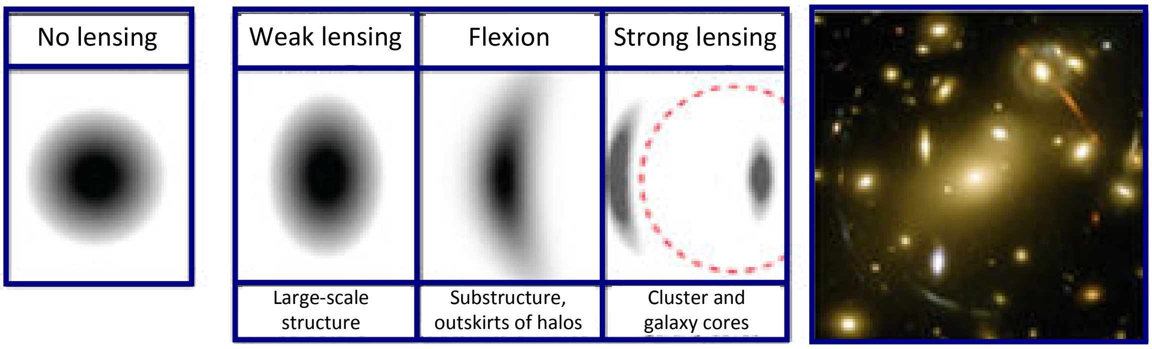

Figure 1. Gravitational lensing on a circularly symmetrical galaxy (Adapted from [3], Credit for Abell 1669: NASA, ESA, and Johan Richard, Caltech, USA).

3. RADIATION DAMAGE IN THE CCD

3.1 CCD charge transfer

For an image to be read out from a CCD, the photo-generated charge must be transferred through the device. The photo-generated signal is collected and stored under an electrode structure upon which the applied voltages may be varied. Through the appropriate variation of these voltages, one can transfer the charge through the device along the columns in the image section of the CCD to the readout register. The charge can then be transferred in a similar way along the readout register to be measured at the output node [4].

For a standard 2000 × 2000 pixel device, the signal charge may be transferred up to 4000 times; a maximum of 2000 transfers along a column followed by 2000 transfers through the serial register. If the transfer from one electrode to the next is not efficient, the image read out from the device will have undergone shape changes compared to the image originally generated.

3.2 Radiation damage and Charge Transfer Inefficiency (CTI)

The radiation environment in space plays a major role in the performance of a CCD-based imaging system. Radiation-induced damage in a CCD [5-6] can lead to a "smearing" of the signal-charge along the direction of charge transfer through the device. This "smearing" of the signal leads to shape changes in the images produced, adding to the shape changes caused by WGL for which the mission is designed to measure. One must therefore be able to either minimise the impact of the radiation damage through the use of optimised operating conditions or use post-processing techniques to remove the "smearing" of the image.

When a high energy proton enters a CCD, several interactions occur, as illustrated in Figure 2. In this study, the interaction of most interest is the displacement damage caused by the interaction of high energy protons in the silicon. The displacement damage produces vacancies in the lattice which will then diffuse until they reach a stable state, such as that shown in Figure 2 with a phosphorous dopant atom in the buried channel.

Charge Transfer Inefficiency (CTI) in a CCD is caused by the capture of signal electrons in traps in the buried channel. The captured electrons may subsequently be released into following charge packets. Traps formed in the buried channel of the CCD have a detrimental impact on the efficiency of the charge transfer through the device. This capture and release of signal-electrons by traps can be modelled using Shockley-Read-Hall theory.

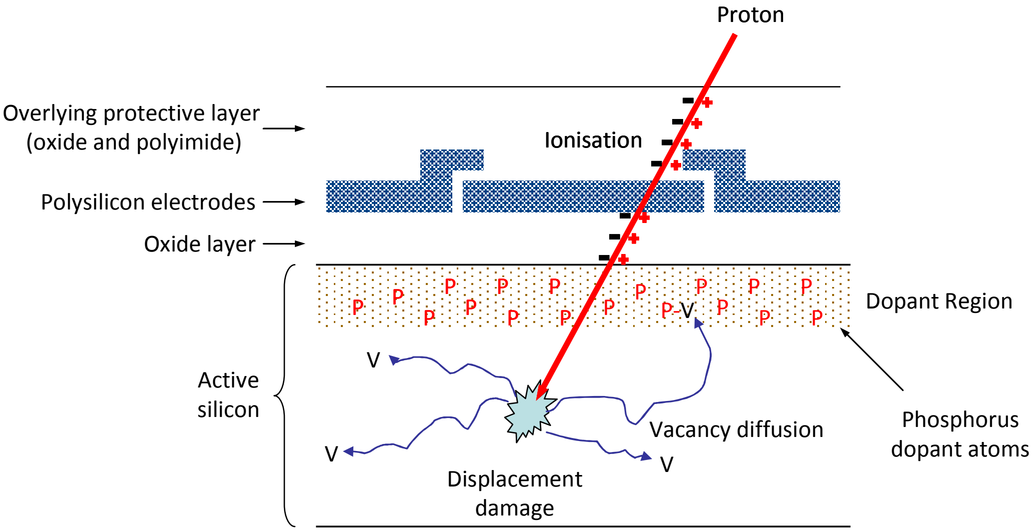

Figure 2. Radiation damage mechanism for a high energy proton in a CCD (adapted from [7]).

4. SHOCKLEY-READ-HALL PARAMETER SPACE

4.1 Shockley-Read-Hall theory

Shockley-Read-Hall theory [8] can be used to model the capture and release of electrons in a CCD through the use of two exponential time constants. The probability of electron capture P_c (Equation 1) is dependent on the dwell time t and the capture time-constant τ_c (Equation 2), a combination of the capture cross-section σ, the electron density n at the trap site and the thermal velocity v_{th} (Equation 3) of the electrons (dependent on the temperature T), where m_e^* is the effective electron mass. The dwell time t may be defined as the time during which the charge packet remains in the same position. The probability P_e of the emission of an electron from an occupied trap in a time t (Equation 4) is dependent on the emission time constant τ_e (Equation 5), which is dependent on the energy level of the trap E. These equations can be used to determine the dynamics of the capture and release of signal-electrons in the CCD, provided one uses an appropriate set of parameters to define the different trap species present.

$$P_c = 1 - \exp\left(-\frac{t}{\tau_c}\right) \quad (1)$$

$$\tau_c = \frac{1}{\sigma n v_{th}} \quad (2)$$

$$\frac{1}{2} m_e^* v_{th}^2 = \frac{3}{2} kT \quad (3)$$

$$P_e = 1 - \exp\left(-\frac{t}{\tau_e}\right) \quad (4)$$

$$\tau_e = \frac{1}{\sigma N_c v_{th}} \exp\left(\frac{E}{kT}\right) \quad (5)$$

4.2 Shockley-Read-Hall parameter space

The parameter-space specified by Shockley-Read-Hall theory defines each trap species through the capture and release time constants. Accurate specification of the required parameters is essential for the modelling of the charge capture and release mechanisms. One must consider not only the energy level of the trap E and the capture cross-section σ, but also the trap density and the electron density at the trap site. The parameter system is, however, complicated by the degeneracy of the system and it can be difficult to separate the parameters experimentally. For example, an over estimation of the electron density at the trap site by a factor of two, coupled to an under estimation of the capture cross-section by a factor of two will yield the same capture dynamics as that achieved through the use of the correct values. For this reason, the parameter selection when modelling radiation-induced damage in a CCD is a complex process.

4.3 Capture and release: the "smearing of the image".

The dynamics of the capture and release of charge, Figure 3, determine the efficiency of the charge transfer through the CCD. As charge passes through the buried channel in a CCD it may encounter a trap, Figure 3A to 3B. In the second state, Figure 3B, a single electron may be captured by the trap and removed from the charge packet, with the probability of capture dependent on Equation 1. When the captured electron is subsequently released, as defined by Equation 4, if the charge packet from which it was released has only moved on one position, Figure 3C, the electron returns to the charge packet from which it was captured and there is no net charge loss from this packet. If, however, the captured electron remains trapped for a longer period of time, then the charge may be deposited into one of the following charge packets, Figure 3D, resulting in reduced Charge Transfer Efficiency (CTE) and a "trail" of charge. This effect leads to an effective "smearing" of the image, changing the shape of any objects in the image.

The balance between the occurrence of Figure 3C and Figure 3D is dependent on the dwell time beneath each electrode and the parameters of the trap involved. Through the careful optimisation of the timings and operating parameters, the CTI can be minimised [9]. However, some degree of CTI may still be present, particularly following high doses of irradiation (an increased density of traps) such as those encountered in orbit.

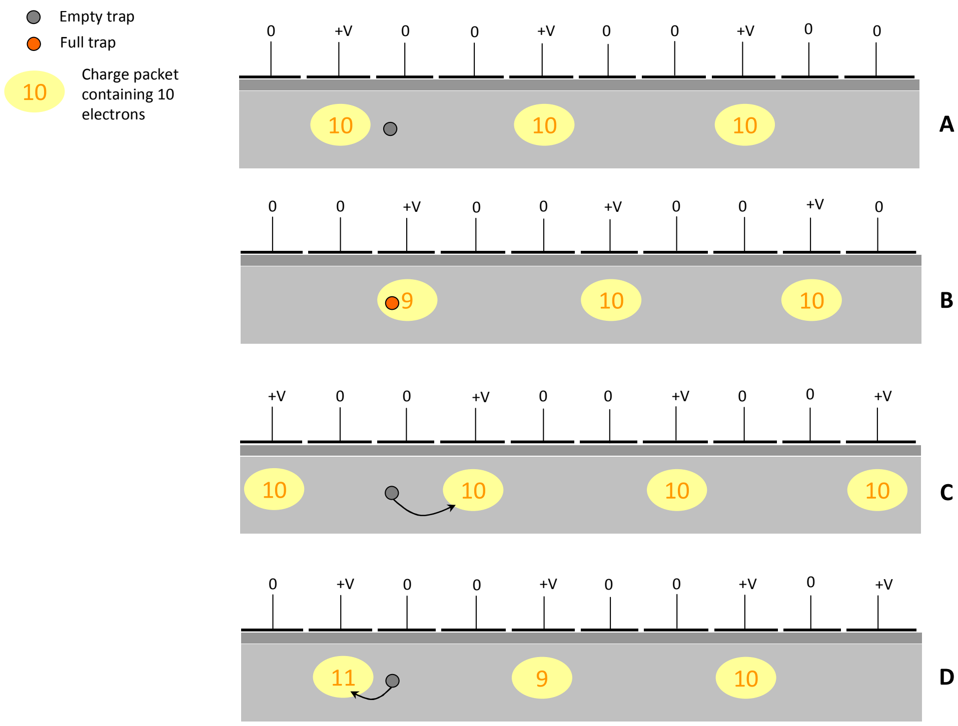

Figure 3. The capture and release dynamics as charge is transferred through a CCD. Time is shown to be increasing down the figure from A to D. Figure taken from Hall, 2012.

5. MONTE CARLO MODEL OF CCD CHARGE TRANSFER

There are many aspects to be considered when designing a Monte Carlo model of charge transfer in a CCD. Here, we consider in more detail the parameter selection, the implementation of the clocking mechanism and the incorporation of a physical charge storage model. Each aspect of the model will be considered in the following sections of the paper, following a brief overview of the simulation structure.

5.1 Basic simulation structure

The simulation has been programmed in C++ and uses a series of arrays to handle the signal-charge and traps. The traps are randomly placed throughout the "trap arrays" at the start of the simulation and then remain in place throughout all transfers, with Shockley-Read-Hall theory used to determine capture and release from the "signal-charge array". Whilst full details of the simulation are not given here, the three main aspects of the simulation have been treated with what was thought to be the most physical method and are discussed in Sections 6-8.

6. PARAMETER CHOICE AND VALIDATION

6.1 Parameter selection

Following the decision to provide a "physically accurate" model of charge transfer in the CCD, the initial trap parameters were selected based on experimental measurements from [10]. Various methods can be used to determine the physical trap parameters, such as the analysis of time constants of exponentially decaying charge tails. Although many trap parameters can be determined through experiment, the calculation of the trap density requires a knowledge of the charge storage characteristics in the device in question, namely the signal-volume characteristics. For this reason, the trap density has been optimised such that the simulated results are consistent with experimental CTI data using single pixel events from Mn-Kα X-rays.

The parameters used in the simulation are given in Table 1, detailing approximate relative trap densities and emission time constants at -114°C. Using parameters based on physical measurements, as opposed to parameters based on a best-fit approach to the experimental data, a change in the operation of the CCD such as a change in temperature or change in the clocking scheme, should not require a change in the trapping parameters. Due to the degeneracy of the parameter space, it is possible (when using a best-fit approach to experimental data) that the trap parameters chosen may be one of many "minima" found in the fitting process and not a truly physical parameter set. Whilst these parameters may offer a consistent result under one set of conditions, the results may not be valid following a change in the experimental conditions such as the temperature or clocking scheme.

6.2 Parameter space

Taking the trap parameters as detailed in Table 1, the emission time constants of the traps can be considered across a range of temperatures, Figure 4. The dwell time of a charge packet under each electrode must be compared to the emission time constant when one considers the impact on CTI, as discussed with reference to Figure 3. For example, with a dwell time of 10^{-4} seconds and temperature of 160 K, the dominant trap species is $(V\text{-}V)^{--}$ whilst other trap species will either remain filled following capture (e.g. Si-E) or release their captured electron back into the charge packet from which it was removed (e.g. Si-A).

Table 1. The basic physical trap parameters implemented initially in the simulation at -114°C, based on experimental measurements from [10].

Trap	Energy (eV)	σ (cm^2)	$N_t^{relative}$	τ_e (s)
Si-E	0.46	5×10^{-15}	5	1849
$(V\text{-}V)^-$	0.41	5×10^{-16}	1	481
Unknown	0.30	5×10^{-16}	1	156×10^{-3}
$(V\text{-}V)^{--}$	0.21	5×10^{-16}	1	220×10^{-6}
Si-A	0.17	1×10^{-14}	10	0.59×10^{-6}

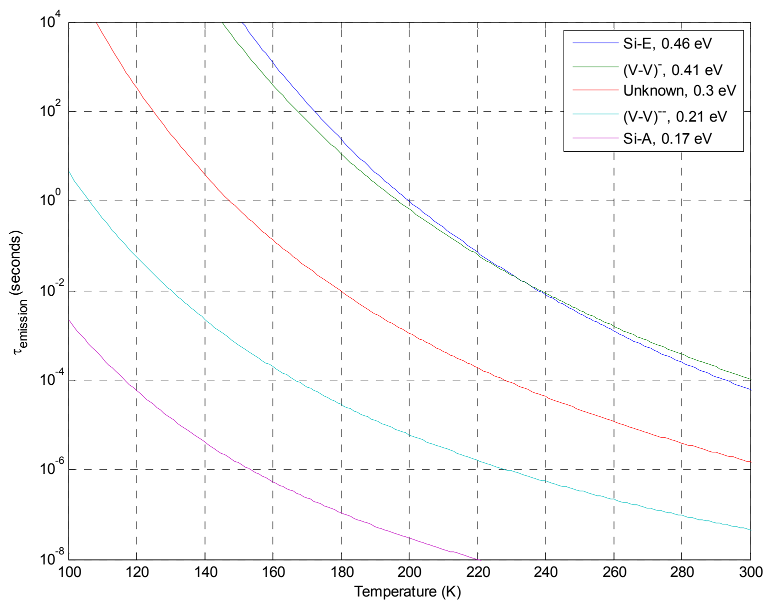

Figure 4. Temperature dependence of the emission time constant for the five trap species used [11].

Although in the past the operating temperature has often been chosen as the operational parameter to vary to optimise charge transfer efficiency, this is not the only experimental parameter that can be used. Section 7 details the optimisation of the clocking scheme to provide a dwell time that minimises the charge loss (maximising the probability of Figure 3C and minimising the probability of Figure 3D).

6.3 Validation of the model: Part I

The initial method of validation of the model, combining the appropriate calibration of the trap densities was performed through a simulation of the same experimental technique as that used to calculate the CTI in the real devices. Taking a series of images of Mn-Kα X-rays, all spatially separated by an appropriate number of pixels, one can produce a plot of the peak signal in a single pixel event against the number of pixels through which the signal has passed. Taking a line of best fit through this plot provides a measure of the CTI (the proportion of charge lost per pixel transfer), Figure 5. The results from the simulation were found to be consistent with the experimental results, Table 2 and Table 3. Whilst this technique provides suitable measures for validation of charge capture and release (combined with a study of charge tails), for each parameter set, several thousand runs of the simulation are required to provide sufficient data to allow the removal of the Monte Carlo noise.

If an analytical approach was taken in which the result was constant from one run to the next through the use of mathematical equations to calculate the charge loss, then the trap parameters could be iterated to give a "best-fit" parameter set. However, as discussed above, although the parameters may provide a simulation that can reproduce the effects of radiation-induced damage under those specific conditions, the physicality of the chosen parameters should be questioned, particularly with regard to the many minima that may be found with such an iterative process. Here, in the Monte Carlo approach, it should also be noted that an iterative process to determine the trap parameters is not practical due to the running times required for each parameter-set tried.

Table 2. The experimental and simulated parallel CTI for two different background levels, 10 MeV proton fluence of 5×10^9 protons cm^{-2} [11].

Conditions	Experimental CTI	Simulated CTI
No background	$2.3\pm0.1 \times 10^{-4}$	$2.2\pm0.2 \times 10^{-4}$
$50e^-$ optical background	$1.3\pm0.1 \times 10^{-4}$	$1.4\pm0.2 \times 10^{-4}$

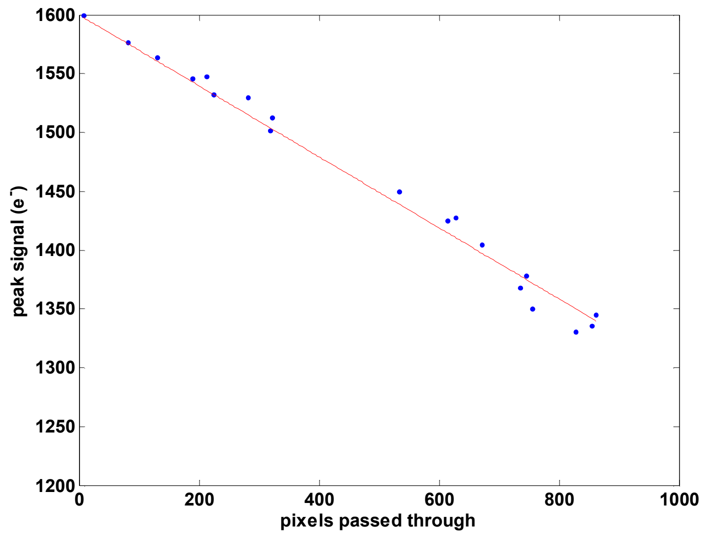

Figure 5. Plot of peak photon intensity versus position for Fe-55 X-ray events in the detector in photon counting mode. A best fit to the peak signal at positions across the CCD can be used to determine the CTI (here ~2×10^{-4}).

Table 3. The experimental and simulated serial CTI for two different background levels, 10 MeV proton fluence of 4×10^{9} protons cm^{-2} (different to the parallel case due to the device and experimental technique used) [12].

Conditions	Experimental CTI	Simulated CTI
No background	$3.8 \pm 0.2 \times 10^{-5}$	$3.8 \pm 0.4 \times 10^{-5}$
$90e^{-}$ optical background	$3.4 \pm 0.2 \times 10^{-5}$	$3.1 \pm 0.3 \times 10^{-5}$

7. CLOCKING IMPLEMENTATION AND IMPACT

7.1 Clocking implementation

The methods used to implement the clocking scheme into the charge transfer simulation must allow flexibility such that the clocking scheme can be changed (whilst still providing results consistent with the experiments) and no other parameters require alteration. In this simulation, the clocking scheme, Figure 6 (top) is split into a series of "phases". Each phase corresponds to a change in the clocking scheme, such that, in this example for the parallel transfers, there are 8 phases. Each phase is programmed independently, with volumes altered accordingly (Section 8). Emission and capture are considered for each "phase" consecutively as the charge is passed through the device. With the appropriate initial physical trap parameters, changes to the clocking scheme should therefore not require further parameter alterations.

7.2 Variations in serial register clocking

It has recently been shown in [12] that, with a physical set of trap parameters and clocking scheme implementation, the clocking scheme can be optimised to minimise CTI. Through the consideration of two different serial register clocking schemes, burst and video modes as shown in Figure 7 (top) and Figure 7 (middle) respectively, the simulation has been tested with regards to the consistency with the experimental results, demonstrating simulated CTI values within 10% of the experimental values. Using the simulation alongside an analytical approach for a simplified trapping solution in the serial register (taking the approximation that the Si-A dominates), the best-case clocking scheme was predicted. The simulation demonstrated a potential improvement in CTE of 26%. The experimental data produced following this prediction demonstrated an improvement in serial CTE of 20%, consistent within the trap species approximation made, Figure 8.

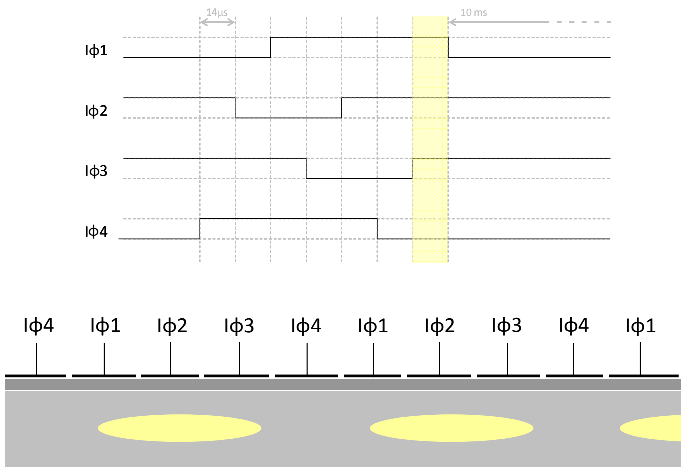

Figure 6. The clocking scheme (top) has been split into 8 "phases", each corresponding to a change in the location of the charge packet under the electrodes. The position of the charge packet (highlighted) in this case is shown (lower).

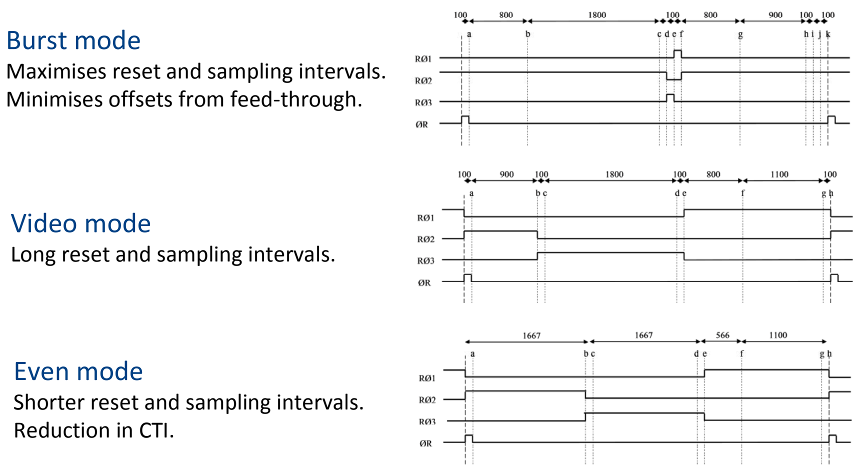

Figure 7. Burst mode and video mode clocking schemes as tested experimentally and subsequently simulated. The third scheme, "even mode", was predicted to provide the best-case CTE following simulations, [12].

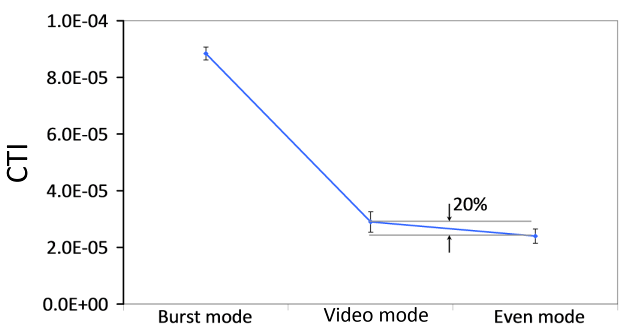

Figure 8. The experimental results from using the three clocking schemes shown in Figure 7, demonstrating the improvements made through the prediction of an optimised clocking scheme, [12].

8. SIGNAL-VOLUME MODELS

The parameters required for Shockley-Read-Hall theory, as specified in Section 4, include the electron density *n* at the location of the trap. This parameter has previously been the subject of much debate, with various models discussed from constant density to constant volume implementations. In order to keep the Monte Carlo simulation as physical as possible, the Silvaco software package has been used to model the charge distribution in three dimensions, [14].

8.1 Signal-Volume modelling in Silvaco

The Silvaco package [13] allows the three-dimensional modelling of charge distributions in a CCD pixel. Here, a pixel from the CCD proposed for use in Euclid at the time of simulation has been modelled with a two-dimensional plane through the three-dimensional structure shown in Figure 9.

8.2 Density profiling

The three dimensional charge storage structure discussed above cannot be placed directly into the Monte Carlo simulation due to limitations on running time and computational power available. Therefore, one must convert these data into a form that may be used in the charge transfer simulation. The process of "density profiling" used involves the conversion of the charge storage data into a "one dimensional volumetric model". Taking a "cut" through the 2D plane, one can create an electron concentration plot for the *x*, *y* and *z* axes of the CCD, shown for one dimension in Figure 10.

8.3 Current implementation

In the current implementation of the charge transfer model, a density profile is taken in each dimension. Through the combination with the trap parameters and using Equations 1 to 5, this density profile can be converted into a probability profile for each trap species and for each dwell time in the clocking scheme "phases". In this way, a "cut-off" probability of capture can be selected and this relates to a "distance" in each dimension inside of which all traps are considered to encounter electrons with sufficient density to capture; outside of this volume the electron density is considered too low for capture to occur. Through the multiplication of the capture distances in all three dimensions, a "capture volume" is produced inside which traps will capture and outside of which no capture will occur. A "signal-volume" model, of which an example is given in Figure 11, must be created for each dwell time and trap species. The use of this "binary system" for capture allows the implementation of physical signal-volume characteristics whilst maintaining reasonable operating times.

The simulation output using this model has been compared to fractional charge-loss data taken experimentally [15] in the signal range of 10-40,000 electrons and has been found to produce consistent results, Figure 12. Although this signal-volume model is consistent with the experimental data, if one considers a non-binary approach the results may be further improved for small-scale effects.

9. FUTURE MODEL DEVELOPMENT

9.1 Signal-Volume enhancements

To improve upon the "binary" approach discussed above, a variable capture probability must be considered. One such method of improvement involves the consideration of the probability-profile at several cut-off capture probabilities to provide a stepped signal-volume profile, Figure 11. The use of such a profile would allow a variable trapping probability to be considered whilst maintaining the physicality of the approach and the low-computational requirements for the practical operation of the simulation.

9.2 Further validation

The Monte Carlo charge transfer model has been validated against X-ray CTI data, charge tails and the fractional charge loss technique. In all cases, the simulation has been found to be consistent with the experimental data. However, in practice the simulation is designed to allow investigation of the radiation-damage induced shape changes to objects in images to allow the separation of these changes in ellipticity from those caused by WGL. To this end, the next stage in the model validation requires the comparison of simulated galaxy objects with experimental results of the same form. For this purpose, a customised optical test bench is under construction to facilitate the production of suitable images for comparison to the Monte Carlo charge transfer simulated output [16].

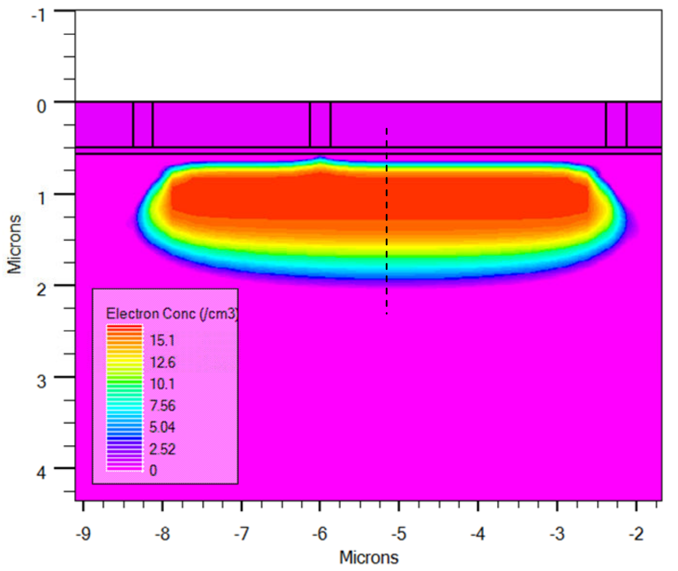

Figure 9. An example 2D plane through the 3D simulated pixel structure of the CCD, showing the charge stored under two electrodes. Adapted from [14].

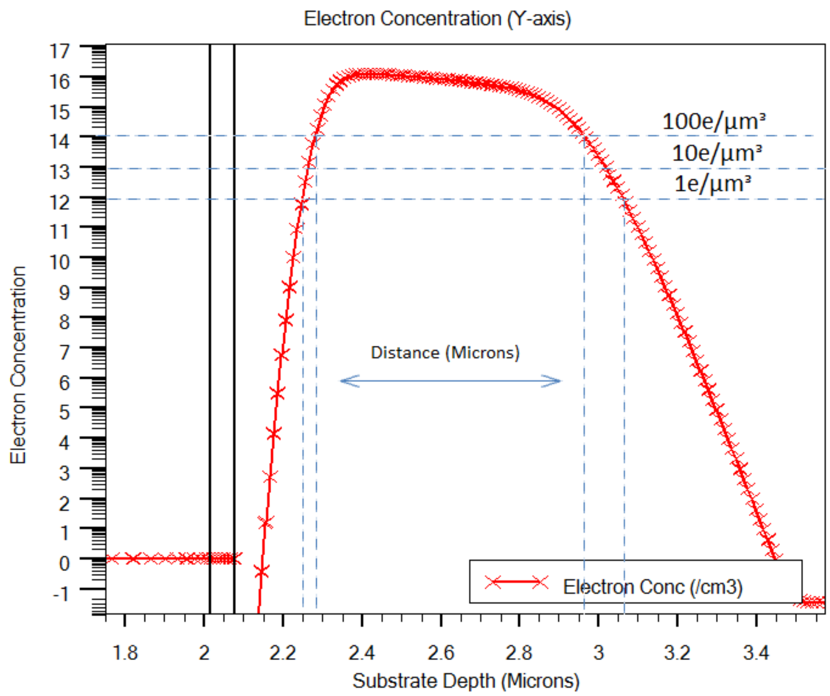

Figure 10. An electron density profile in one dimension of the CCD pixel. Relative electron concentrations are included for 1 e/µm^3, 10 e/µm^3 and 100 e/µm^3 for ease of reference. Adapted from [14].

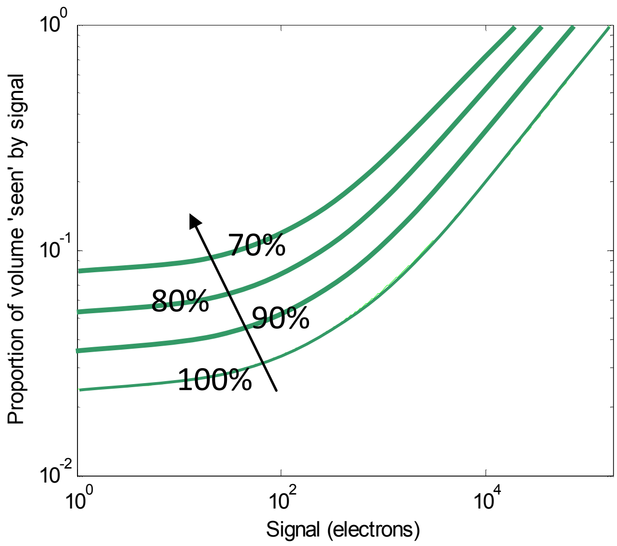

Figure 11. The "signal-volume" model for one trap species and dwell time can be taken to be set at one "cut-off" probability at which the probability of capture is approximated to 100%. The volume of the signal charge packet, normalised against the volume occupied at Full-Well Capacity (FWC), details the volume in which a trap will capture and electron; inside this volume the probability of capture is approximated to 100%. Outside of this volume, a trap is considered to encounter an electron density too low to capture. A variable probability signal-volume model in which the probability of capture is approximated to set values (shown in steps of 10% here) based on a varying density cut-off level could be incorporated into a future implementation (see Section 9).

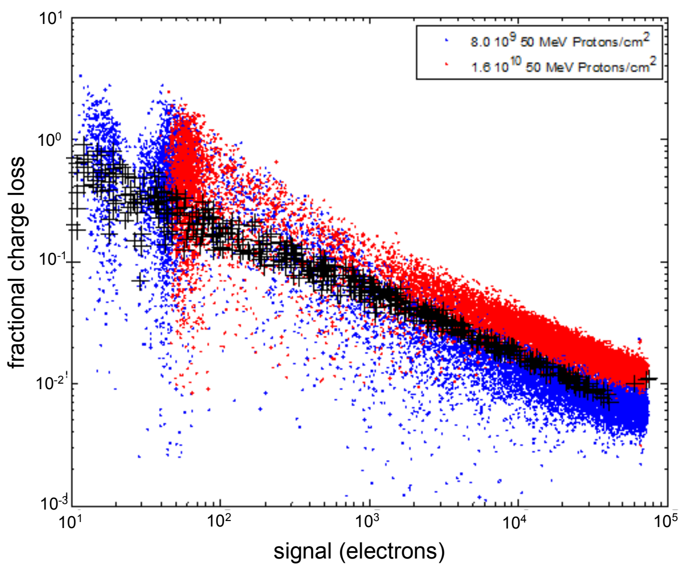

Figure 12. Plot of fractional charge loss measurements produced experimentally (dots) [15] with a charge injection delay of 200 ms, line dwell time of 2 ms and temperature of -130°C for two different proton fluences. The simulated results (crosses, calculated for a mid-range fluence) are shown to demonstrate the same trend as the experimental data across all signal levels, demonstrating the consistency of this signal-volume methodology with the physical results provided experimentally [11].

10. CONCLUSIONS

As the demands on camera performance increase, the impact of radiation-induced damage to the CCD becomes ever more important. To this end, the impact of the damage must be reduced and any remaining effects of the damage must be removed through post processing. A Monte Carlo charge transfer simulation for a radiation damaged CCD can be used to both optimise the operational parameters of the device and aid in the development of algorithms to remove the remaining radiation damage-induced effects. Using a "physical" approach to the operation of the simulation and in the development of the parameter set has produced a simulation that has been successfully validated against experimental X-ray CTI data, charge tails and first pixel response data. Through the use of this approach, the simulation has been used to determine an optimised clocking scheme for the serial register of the CCD, with the results backed with experimental data. This has been achieved through a change only in the clocking scheme and related trapping volume. In the future development of the model, more physically accurate signal-volume model implementations have been suggested to improve the performance of the simulation in terms of small-scale effects.

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