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In situ trap parameter studies in CCDs for space applications

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ABSTRACT

Charge-Coupled Devices are the detector of choice for the focal planes of many optical and X-ray space telescopes. In recent years, EM-CCDs, SCDs and CMOS sensors have been used, or baselined, for missions in which the detection of X-ray and visible photons are key to the science goals of the mission. When placed in orbit, silicon-based detectors will suffer radiation damage as a consequence of the harsh space radiation environment, creating traps in the silicon. The radiation-induced traps will capture and release signal electrons, effectively "smearing" the image. Without correction, this smearing of the image would have major consequences on the science goals of the missions. Fitting to observed results, through careful planning of observation strategies while the radiation dose received remains low in the early stages of the mission, has previously been used to correct against the radiation damage effects. As the science goals becoming increasingly demanding, however, the correction algorithms require greater accuracy and a more physical approach is required, removing the effects of the radiation damage by modelling the trap capture and release mechanisms to a high level of detail. The drive for increasingly accurate trap parameters has led to the development of new methods of characterisation of traps in the silicon, measuring the trap properties and their effects to the single-trap level *in situ*. Here, we summarise the latest developments in trap characterisation techniques for n-channel and p-channel devices.

Keywords: CCD, trap, silicon, defect, radiation damage, n-channel, p-channel, pocket pumping, Euclid, Gaia, HST, CTI

1. INTRODUCTION

For many years, the detector of choice for use in the focal plane of optical and X-ray telescopes, whether on the ground or in-orbit, has been the Charge Coupled Device (CCD) or a similar silicon-based technology. CCDs offer high sensitivity and high resolution imaging and spectroscopy of both optical and X-ray photons and Electron Multiplying (EM) CCDs are now being increasingly investigated for use in space applications [1].

Despite the advantages that CCDs offer, when used in space they are often subjected to a harsh radiation environment and this can cause damage to the silicon lattice in the devices. This damage takes the form of defects in the lattice which lead to the formation of additional energy levels situated between the valence and conduction bands in the silicon band structure. These energy levels, each with their own electron capture and emission characteristics, act as traps that capture and release signal charge as it is transferred through the device. It is this capture and subsequent release of the signal charge that leads to an increasing level of smearing in the images taken in the focal planes as the time in orbit increases.

It has been demonstrated in orbit with Hubble in 2010 that this "smearing" of the image can be corrected to the 97% level [2] using a pixel-based correction algorithm, improved over the original 90% correction achieved in 2006. For the ESA Gaia mission [3], a Charge Distortion Model has been developed [4] that satisfies the limits set for the data correction required by the mission. Both models make use of emission time constants for each of the trap species that is modelled. The accuracy of these trap parameters plays a major role in determining the accuracy of the simulation and therefore the quality of the correction applied.

As the science goals of missions increase in complexity and as the requirements placed on the detectors forming the focal plane become ever more demanding, the importance of accurate correction is becoming increasingly significant. As an example, the ESA Euclid mission VIS instrument [5][6] will require correction against the radiation induced "smearing" of the signal an order of magnitude stronger than the 90% originally achieved with Hubble [7][8].

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Current correction techniques make use of trap parameters that are, on the whole, taken from measurements of the average properties of trap across a whole device or series of devices. These parameters have been shown to provide the correction required in current usage, however, moving forwards it becomes increasingly important to investigate trap properties at the single-trap level, pushing the boundaries of the analysis and correction techniques to new heights. It is for this reason that in-situ single-trap studies are of vital importance. Using methods developed as an extension to pocket-pumping techniques we demonstrate how, through the use of specific clocking schemes at appropriate temperatures, it is possible to study the properties of individual defects in the silicon lattice in high levels of detail.

2. POCKET PUMPING

For over 20 years, the technique of pocket pumping has been used to investigate and characterise traps in CCDs [9]. The technique allows the characterisation of electron traps down to the single electron level and also allows the investigation of "statistical traps which may or may not capture an electron" [9]. The technique is described in greater detail in [10] for the case of design traps and process traps, i.e. traps that are formed during the manufacture of the device and bulk traps caused by intrinsic defects in the lattice.

The pocket pumping technique requires the exposure of the CCD to a flat field of several thousand electrons followed by the clocking of the signal back-and-forth across several lines in the device. If the charge passes over a trap during the transfers then it is possible that some of the signal electrons may be captured. Some time later during the transfers, the trapped electron(s) will be released and if the captured electron or electrons are released into a different charge packet from that in which they were captured the signal is said to have been "pumped". The continued "pumping" in the presence of a trap gradually removes signal at the trap site and moves this captured signal into another image pixel, creating a dipole in the image at the same location as the trap itself.

The pocket pumping technique has been demonstrated in [10] to allow the characterisation of bulk traps in a CCD. Using this method, it has been shown that single electron bulk traps in the device can be measured in a device. Whilst the method is able to demonstrate the presence, location and size of the trap, it does not offer further characterisation of the more detailed properties of the traps, such as the emission time constant for the release of a captured electron in the defect and the capture dynamics. In order to characterise the traps to the level of detail required to allow the accurate correction of images, one must develop the technique further.

Traps in silicon are not confined to those present before and immediately following manufacture, however, as further defects can result from the irradiation of the devices. The radiation environment in some space-based applications of the devices can be particularly harsh and it is in such environments that full characterisation of the traps is essential to allow the correction of the images against the smearing detailed above.

3. RADIATION INDUCED TRAPS

There are many causes of defects in the silicon lattice. Those which have been mentioned above include intrinsic defects that were present in the raw material or those that may have been introduced during manufacture. Under irradiation, however, the number of defects in the device can dramatically increase.

High energy protons dominate the radiation environment for many missions and these high energy protons can cause displacement damage in the device, effectively knocking silicon atoms out of the lattice to leave vacancies. The vacancies themselves are unstable and will diffuse through the lattice until they reach a stable configuration, such as with another vacancy to form the divacancy or with an impurity in the lattice, such as in the formation of the Si-A or Si-E defects, formed from a vacancy with an oxygen or phosphorous atom respectively. Whilst the impact of radiation damage has been studied at great length (e.g. [11][12]), for both n-channel and p-channel CCDs (e.g. [13]), there is still a lot to be learnt about the defects themselves.

There are many known silicon lattice defects that produce traps in a CCD with capture and emission characteristics on the same time scales as the integration and transfer of charge in the device. It is these traps that will interfere most strongly with the images that are being read out and knowledge of the properties of these traps is of particular importance. There are four main dominant traps in the silicon lattice, as shown in Figure 1, noting that the divacancy has

two energy levels in the range of interest for CCD operation, leading to five main energy levels. The parameters used to derive the emission time curves shown in Figure 1 are based on literature values for averaged measurements across many defects in a device(s). It is important to note the temperature dependence of the traps; the traps of most interest will vary depending on the operating temperature of the device. For example, at room temperature the Si-E will have a similar impact as the doubly-negative charge state of the divacancy at approximately 160 K. The relative densities of the different species will vary and, along with other important characteristics such as dark current, the temperature of operation of the device must be chosen carefully. Of course, the more accurately one knows the parameters in question, such as the emission time constants, the better educated the decision will be.
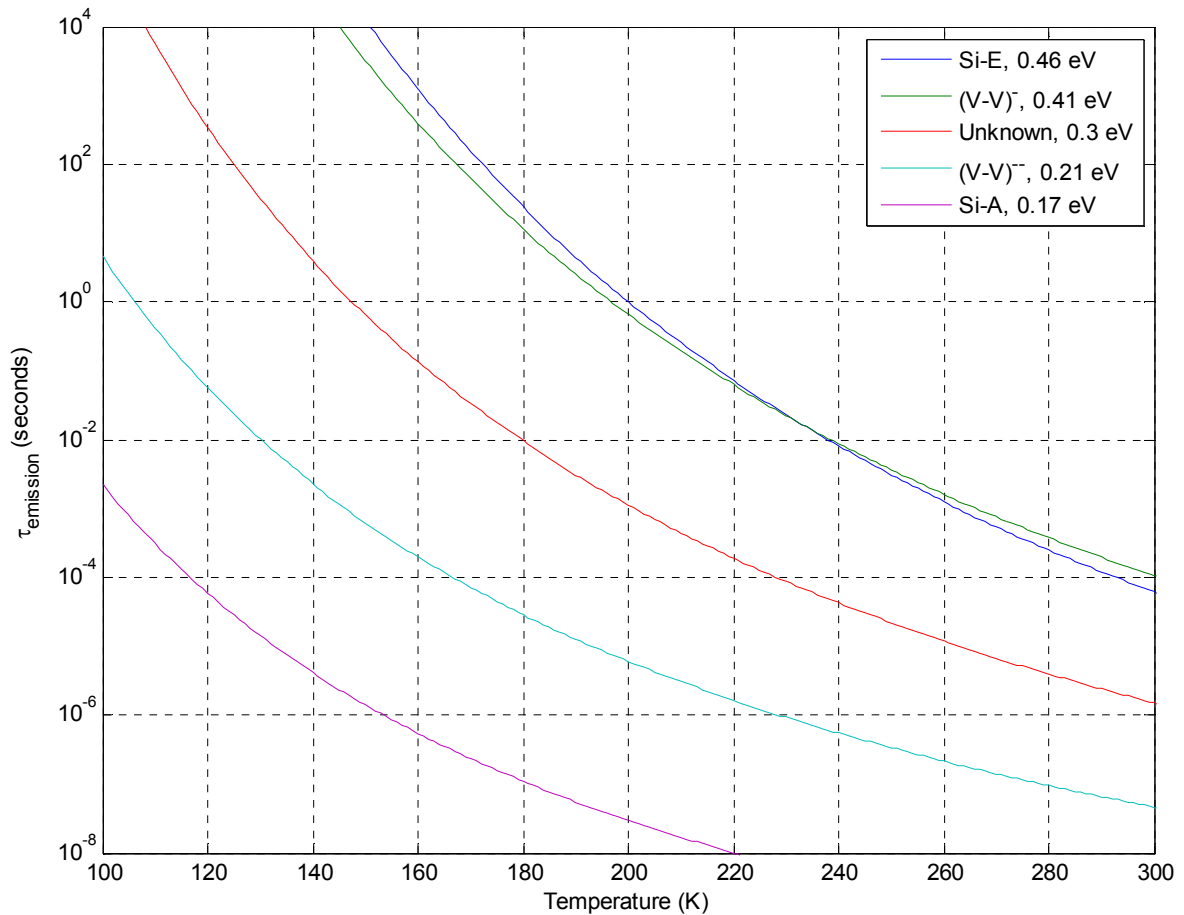
Figure 1. Temperature dependence of the emission time constant for the four main trap species in CCDs. Uncertainties on the emission time constants for the defects shown can be as large as one order of magnitude. [14]

The relevant energy levels for the traps detailed in Figure 1 are shown in Figure 2. Although the position of the average energy levels is thought to be well known, little is known about the spread or distribution of the energy levels within these results and the uncertainties on the measurements are often an order of magnitude or higher in some cases. The emission time constants, which are themselves a function of the energy level of the trap through Shockley-Read-Hall theory [15][16], are one of the most important inputs to the image correction algorithms required for correction against the smearing of images in radiation damaged devices.

Conduction band

Si-A
0.17eV

(V-V)⁻⁻
0.21eV

Unknown
0.3eV

(V-V)⁻
0.41eV

Si-E
0.46eV

Valence band
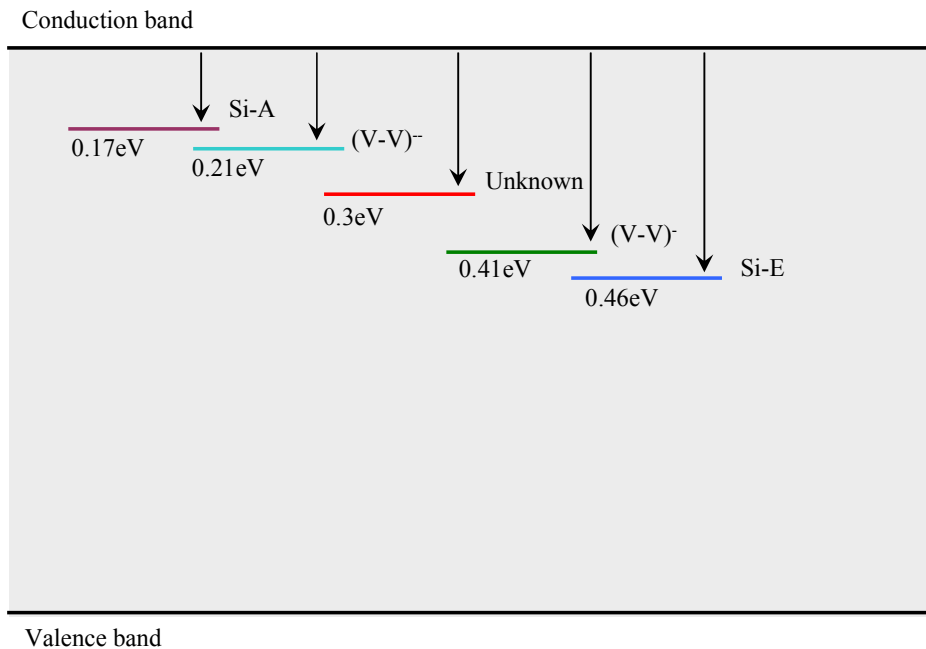
Figure 2. The energy levels of the defects with emission times shown in Figure 1. Although the locations of the energy levels is known for each trap species as a whole, little is known regarding the makeup of the energy level structure at the few percent level. The distribution of energy levels for traps of the same species and possible splitting of the energy levels into several distinct bands is currently not well understood.

4. IMAGE CORRECTION TECHNIQUES

As discussed above, the presence of defects in the silicon lattice of the CCD creates traps that can capture, and later release, signal electrons as they are transferred through the CCD. This leads to smearing of the signal that must be corrected on the ground and therefore there is a great deal of development involved in producing suitable models and algorithms to accurately correct against the radiation-induced damage.

For the Hubble Space Telescope, a correction algorithm has been developed that is able to achieve a 97% correction in data [2]. The algorithm uses forward modelling of radiation damage to progressively correct against the smearing in the images. The model used requires accurate parameters for each trap species incorporated into the system. Within limits imposed by the noise of the detector system, the more accurate the trap parameters the more accurately the model can correct against the radiation damage.

For Gaia, a slightly different approach is used. A Charge Distortion Model has been developed [4] that describes the effects of the radiation-induced traps in a physically realistic manner whilst also providing fast running times. The Charge Distortion Model therefore uses a column-averaged approach, not considering each individual defect in the system but instead concentrating on the average impact of all traps along a column in one calculation.

Despite the different approaches, all models rely on an accurate and complete parameter space. This parameter space includes the emission time constant of the traps incorporated into the models; the more accurate the parameters, the more accurate the correction.

5. REQUIREMENT FOR GREATER ACCURACY

The correction methods described above are only as good as the input parameters. Whilst great strides have been made in accurately determining the charge storage characteristics in devices [17][18] (another vital component in the correction algorithms), in order to achieve the increasingly challenging requirements for space missions it is vital that the detailed knowledge of the traps species and their parameters is improved. With these increasing demands it is becoming more important to consider not only the averaged impact of many traps across a device but more so to consider the impact of traps at the individual level [19]. Whilst for Hubble the correction is able to counteract radiation induced smearing to the 97% level, Euclid will require correction at the 99% level [5][7][8]. To this end, moving forwards for future missions will require trap parameters to be known to uncertainties of a few percent or less. This can only be achieved by examining defects at the single-trap level using techniques such as pocket pumping and by gaining a deeper understanding of the defects through interdisciplinary studies, such as with Hybrid Density Functional Theory, as has been instigated in [20] and [21].

6. THE "SINGLE TRAP PUMPING" TECHNIQUE

Although pocket pumping, as described in Section 2, can locate individual traps in a CCD, further development of the pocket pumping method has been required to look at individual traps through "single trap pumping" [22][23]. The "single trap pumping" technique as a method to accurately determine individual trap parameters has been described in great detail in [24]. In summary, the technique uses a specific clocking sequence to transfer charge from one pixel to the next (i.e. phase 1 to phase 1 and not over several lines in the device), Figure 3.
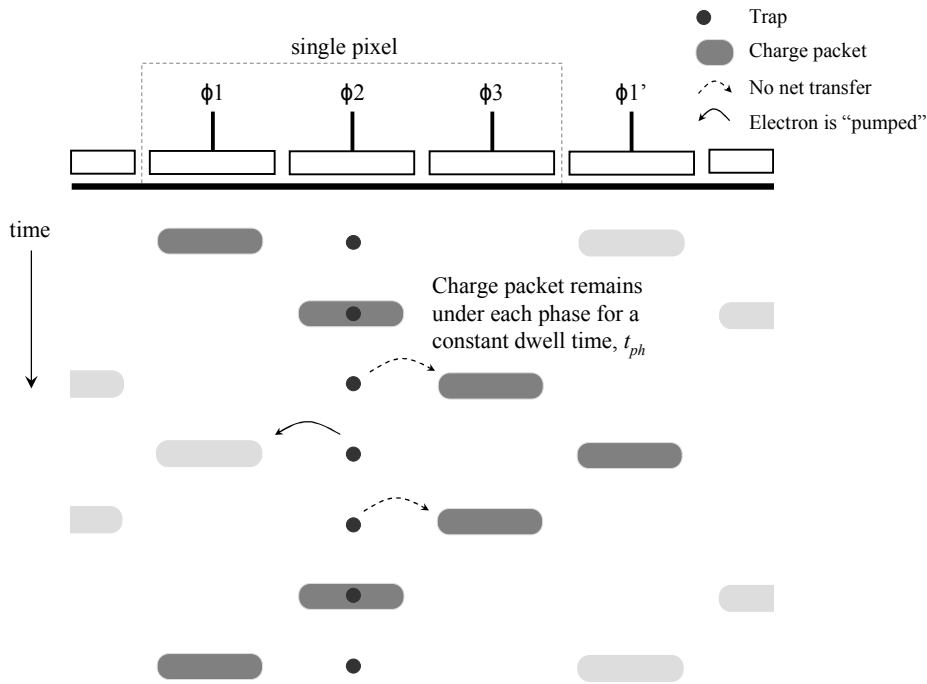

Figure 3. A flat field is integrated in the device, either from an external light source or from an "internal" method such as described in [25], with the charge packets then being shuffled from to phase 1 in the neighbouring pixel and back again. The charge packets rest under each phase for the same dwell time, t_{ph}. After a set number of pumps (*e.g.* 1000), the image is read out. The process is then repeated with a new dwell time, building a series of images with increasing dwell times. Dipoles will be seen in the image at trap sites and by tracing the amplitude of these dipoles through the varying dwell times one is able to accurately determine the trap emission time at the single-trap level with the device under the exact operating conditions as would be used in orbit.

This clocking sequence maintains a constant dwell time under each phase for each measurement taken. A flat-field of signal is "pumped" from, for example, phase 1 in the first pixel to phase 1 in the neighbouring pixel and back, with this being defined as one pumping cycle. Repeating this process over many pumping cycles, typically several thousand cycles in total, leads to the formation of dipoles the image at locations where a trap has actively transferred signal from one pixel to the next, much in the same way as those formed in the standard pocket pumping process.

The above process can then be repeated for a series of different dwell times such that a series of images is produced tracked through different dwell times under each phase. By plotting the intensity of the dipoles tracked across a series of dwell times the trap capture and emission can be probed in the time-domain. In the presence of a trap a characteristic curve is produced. By fitting the curve from Equation 1, where N is the number of pumping cycles and t_{ph} is the clock width, the capture probability (to a first approximation) and the emission times constant of the trap, P_c and τ_e respectively, can be found for each individual trap (derivation and further explanation can be found in [24]).

$$I = NP_c \left(\exp\left(\frac{-t_{ph}}{\tau_e} \right) - \exp\left(\frac{-2t_{ph}}{\tau_e} \right) \right)$$

(1)

During the study of the above detailed technique, we have developed a Monte Carlo simulation of the trap pumping mechanism. The simulation is based on a similar framework to that outlined in [14] and [16], developed further to use matrix manipulation for an increase in the efficiency of the simulation run-time. Using this simulation it is possible to investigate a variety of different scenarios for which the trap locations and full parameter sets are known. An example of four simulated traps is shown in Figure 4.
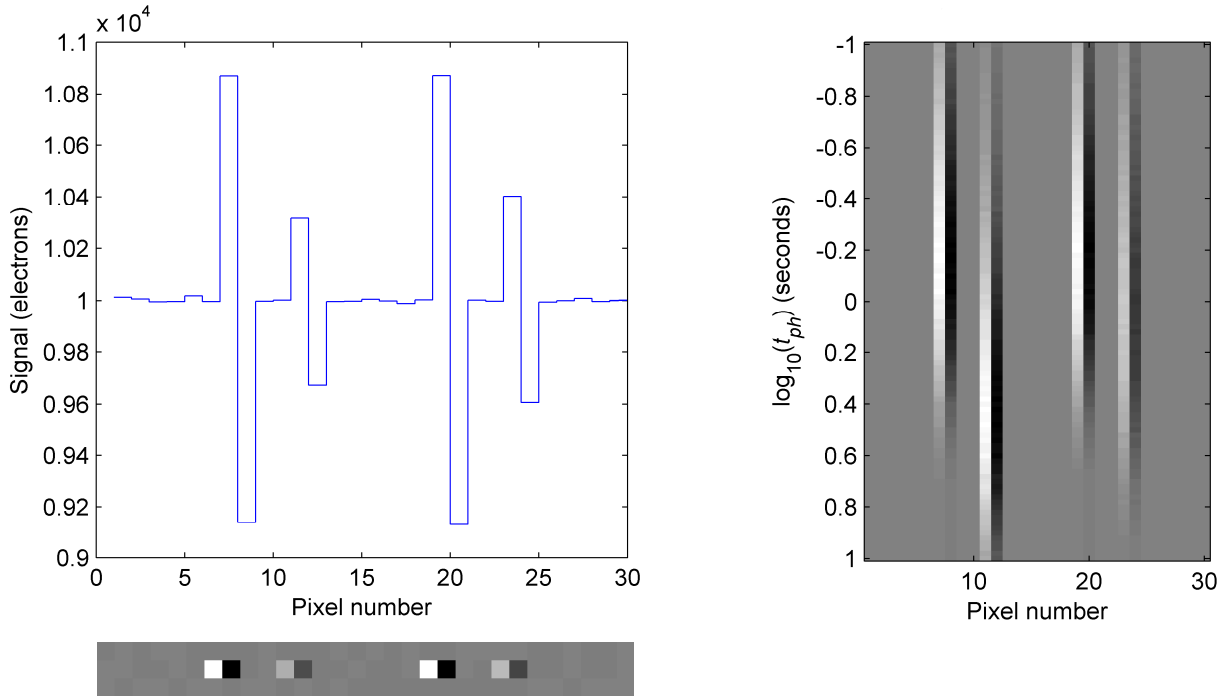
Figure 4. Four single traps simulated with different parameters (described in Figures 5 and 6), pumped with a background signal of 10,000 electrons for 4000 pumping cycles. *Left:* Each trap produces a dipole with an amplitude that is dependent on the trap properties and the clocking width used during the pumping process. In this case, all dipoles are under phase 2 in the device for demonstration purposes, however, if a trap was under phase 3 then the dipole would be reversed (i.e. it would be low-high, reading from left to right). The dipoles as they appear in the simulated image are shown below. *Right:* The cut across the image shown on the left (shown across the *x*-axis) is tracked through a range of clock widths (t_{ph} values) along the *y*-axis, showing the amplitude variation tracing the same form as in Figure 5.

The trap pumping method described above allows the separation of the capture and emission characteristics of single traps in the CCD. By tracking the dipole intensity across a range of clock widths (as shown down the *y*-axis of Figure 4, right) it becomes possible to distinguish between traps with low probabilities of capture (*e.g.* near the edges of the charge packet) at the operating conditions specified, and traps which have a low pumping efficiency (*e.g.* because the operating clock width is not at the peak of the emission time of the trap), Figure 5.
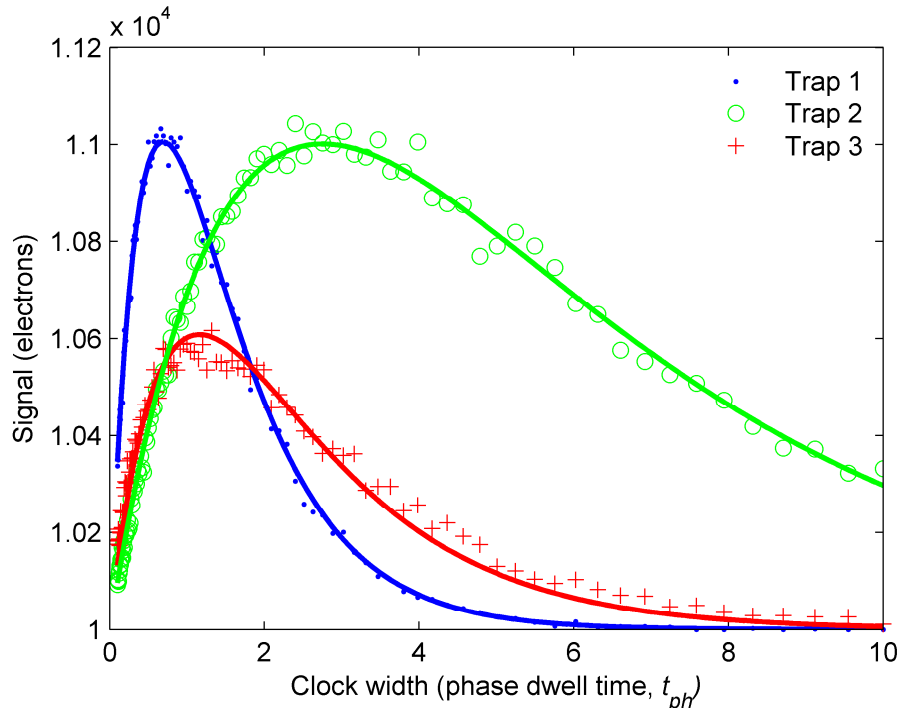
Figure 5. Three simulated traps with varying properties, shown with arbitrary time units. The data points show the results from the Monte Carlo simulation, with the solid lines showing the fit to the data using Equation 1. Traps 1, 2 and 3 have time constants that scale as 1:2:4, showing here how the peaks, and in fact the whole curves, shift in time with varying emission time constants. Traps 1 and 2 have 100% capture probability, whereas Trap 3 has a much lower capture probability. The importance of taking measurements over a range of clock widths is demonstrated if you consider, for example, the results of only pumping with a single clock width where the curves for Trap 1 and Trap 3 intersect; at this point there is no way to determine any differences between the two trap species unless further measurements are taken with varies clock widths. The power of the method is demonstrated in the ability to separate the emission and capture characteristics of each individual trap.

7. IN-SITU TRAP CHARACTERSIATION

We have seen in Section 6 how the trap pumping mechanism operates on a variety of traps with different parameters, demonstrated through the use of simulated results. However, it is of course vital that the technique is demonstrated in practice. It has been demonstrated experimentally in [24] that the technique can be used in an n-channel CCD, in this case using the Si-A as an example, Figure 6. The experimental results show that by using this technique it is possible to discover the emission time constants of single traps in a CCD to within a few percent uncertainty. The parameters of each single trap can be investigated independently (providing the trap density is such that traps are separable between pixels).

It is vital to choose appropriate operating conditions when investigating a trap population or several trap populations. There are two main scenarios that usually occur: knowing the operating conditions but not the relevant trap properties

(i.e. mission specific conditions), or probing the trap species in a device (i.e. aiming to understand the underlying science of the defect populations in more general terms). To allow the relevant trap species to be investigated in either regime, a clock timing width variation of one order of magnitude above and below the appropriate clock widths is recommended to trace traps that may not be fully efficient under the specific operating conditions but may have an impact on the charge transfer. To investigate the underlying science of the trap, a minimum of three temperatures are required to allow the trap capture and emission characteristics to be tracked and hence allow the calculation of the parameters beyond only the emission time constant (*e.g.* energy level of the trap).

It is important to keep in mind, however, the limitations of the drive system being used to operate the device under test and the CCD itself. There will be limitations (both from the electronics and the device itself) at the faster end of the scale in terms of producing effective clock wave forms and there will be limitations at the slower end of the scale as to what is practical (*e.g.* 4 000 pumps with a 20 second t_{ph} will require 1 week of operation for a single data point, however, the same number of pumps with 1 ms t_{ph} will take under 30 seconds). The process can be easily automated to scan a range of clock widths to allow the investigation of many trap species.

The technique is now being used to further investigate traps and defects in both n-channel and p-channel CCDs, producing interesting lines for further research that will be reported in future publications. The current drive in the study of n-channel devices involves an increase in the statistics to investigate possible energy level splitting or distributions, as intimated in the experimental results of [24]. Further investigation is required into the influence of the capture probability on the technique to determine the direct or indirect correlation between the capture probability and pumping efficiency (given as linear in Equation 1 as a first approximation).
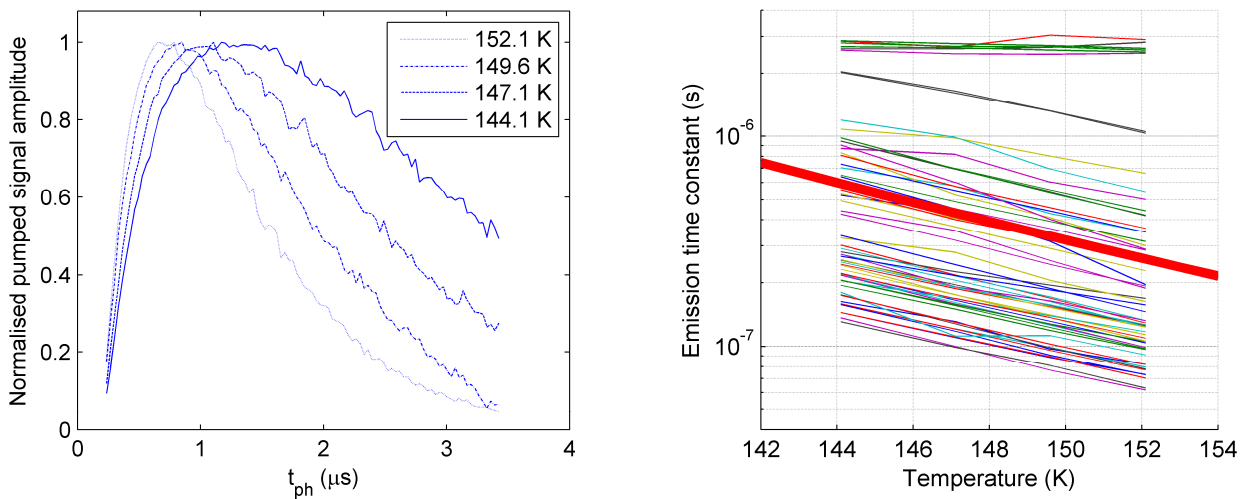
Figure 6. *Left*: One single trap, pumped at four different temperatures, showing the same characteristic curve in these experimental results as those simulated in Section 6. As the temperature decreases, the curve shifts to the right (i.e. with a longer time constant). *Right*: Approximately 60 individual traps pumped at the same four temperatures. Each line details a single lattice defect or trap. The thick line is the theoretical time constant for the Si-A with an energy of 0.17 eV and cross section of 10^{-14} cm^2. Two apparent groupings are seen in the results and these are detailed further in [24], from which this figures was adapted.

8. CONCLUSIONS

The pocket pumping technique has been used for several decades to acquire basic information about defects and traps in CCDs, however, the details about trap properties that can be gained from the standard use of this technique are limited. Through further development of the method, we have demonstrated that the "single trap pumping" method can be used to accurately characterise individual traps with uncertainties of a few percent. Through the use of this new development of the pocket pumping technique, individual defects in the silicon lattice can be located in a device and characterised to unprecedented levels of detail.

As mission objectives become ever more demanding on the focal plane detectors used, there is an increased importance placed on the capabilities of the image correction techniques that act to remove the smearing effects caused by radiation-induced traps. Image correction techniques that are based on models of the capture and release of electrons from traps are limited by the trap parameters used and it is only through gaining a deeper understanding of the traps at the single-trap level that these models can be further improved.

The characterisation of single traps in both n-channel and p-channel devices is ongoing, however, the initial results demonstrate the abilities of the methodology and the benefits that this technique can bring. Through the use of more accurate information about the trap species present, it is possible to not only correct data from orbit, but to optimise detector operation more thoroughly *before* launch [26]. The technique is not only of great interest for ground-based investigations of defects in the silicon lattice but it also has the potential to provide in-orbit real-time information about the individual traps being created in the detectors [22].

9. ACKNOWLEDGEMENTS

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