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Modelling charge transfer inefficiency in Gaia CCDs with in-flight and on-ground data

Saad Ahmed[a], David Hall[a], Jesper Skottfelt[a], Ben Dryer[a], Andrew Holland[a], Cian Crowley[b], and Jose Hernandez[c]

[a]Centre for Electronic Imaging, SPS, The Open University, Milton Keynes, MK7 6AA, UK
[b]HE Space Operations BV for ESA/ESAC, Camino Bajo del Castillo s/n, 28691 Villanueva de la Cañada, Spain
[c]ESA, European Space Astronomy Centre, Camino Bajo del Castillo s/n, 28691 Villanueva de la Cañada, Spain

ABSTRACT

The European Space Agency's Gaia spacecraft was launched in 2013 with the aim of making the largest and most precise map of the Milky Way by taking measurements of almost one billion astronomical objects. It has a focal plane that consists of 106 Charge-Coupled Devices (CCDs), custom designed by Teledyne e2v to help fulfil its objectives. These detectors make measurements of positions, velocities, parallaxes, and other physical properties of any objects, with a sufficiently bright enough magnitude, that pass through their field of view. Operating in space means that the Gaia CCDs have been subjected to radiation damage, both ionizing and non-ionizing in nature, in orbit from predominantly solar radiation. This radiation-induced damage leads to the formation of trap defects in the CCD silicon lattice which can trap electrons during readout leading to the increase of charge transfer inefficiency (CTI) and a reduction in the quality of the returned science data. From previous analysis of in-flight data, the degradation of the CCDs, measured from an increase in CTI, has been calculated to be less that that predicted from pre-flight models and on-ground tests. In this study, in-flight and on-ground data is modelled so that the trap landscapes can be further investigated. This was achieved using a charge transfer model, the Charge Distortion Model (CDM), integrated in the Pyxel detector simulation toolkit. Other simulations, namely C3TM, are used in conjunction with the results from Pyxel to obtain a more thorough understanding of the trap landscape causing the observed CTI effects.

Keywords: CCD, Gaia, Radiation Damage, Pyxel, Simulation, NIEL, Silicon, C3TM

1. INTRODUCTION

The Gaia spacecraft is one of the European Space Agency's (ESA) cornerstone missions, successfully launched in December 2013. Its main goal is to measure the three-dimensional spatial and velocity distribution of stars in the Milky Way and determine their astrophysical properties such as their photometry, and spectra. The large wealth of data should help researchers answer questions about the formation, structure, and the future of the Milky Way. It rotates with a period of six hours, constantly scanning the sky with its two optical telescopes. To date, three Data Releases have been released to the public, detailing the data collected by the spacecraft.[1–4] To help complete its mission objectives, Gaia has a focal plane consisting of 106 charge-coupled devices (CCDs).

1.1 CCDs and the focal plane

Gaia's CCDs were custom-designed and manufactured by Teledyne e2v and were of the CCD91-72 variant. They operate at a nominal temperature of 163K in Time-Delayed Integration (TDI) mode where the CCDs transfer signals continuously at the same rate as the starfield movement across the focal plane; this corresponds to a pixel clocking time of 982.8µs. Each CCD consists of 4500 × 1966 pixels (parallel × serial) of physical dimensions 10 × 30 µm. The CCDs were manufactured in different variants, each used for different instruments across the

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Further author information: (Send correspondence to Saad Ahmed)
Saad Ahmed: E-mail: saad.ahmed@open.ac.uk

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focal plane. They were also manufactured with a number of design features to mitigate the impact of radiation damage. These include a Charge Injection (CI) structure and a Supplementary Buried Channel (SBC) which confines low signals to a smaller volume in the silicon so they encounter fewer traps.[3,5]

2. RADIATION DAMAGE IMPACT

While operating in space, in-flight CCDs become exposed to radiation from different sources which can affect their performance. Gaia in particular, orbits at Lagrange Point 2 (L2) which is a popular orbital position of other missions such as ESA's Euclid, PLATO, and ARIEL space missions. Future missions and research will benefit from a better understanding of L2's radiation environment via the radiation damage impact on the Gaia CCDs. Due to the performance requirements of Gaia, radiation damage on the CCDs was identified as a major factor that would affect the performance and science return of the mission.[2]

When high-energy particles from radiation hit the detectors, they can displace atoms from the silicon lattice leaving behind lattice dislocations termed 'vacancies'. The vacancies diffuse through the silicon lattice and can combine with other vacancies, dopant atoms, or manufacturing impurities in the silicon to form stable states called trap defects. These trap defects form new energy levels between the valence and conduction bands and can capture electrons from signal packets as they are clocked through the area of the defect and release them at a later time on probabilistic timescales, often into a different charge packet. This increases the Charge Transfer Inefficiency (CTI) of the devices which reduces the quality of the data and can lead to trails of charge forming behind the data.[6,7] Depending on which impurities the vacancies combine with, different trap defects can be formed, all of which have different effects on the CTI depending on the devices' operating speed and temperature. The details of these radiation-induced trap defects and their impacts on various space missions has been detailed extensively in the literature.[8,9]

3. PREVIOUS STUDIES

To assess the performance as well as the CTI impact on the Gaia devices, several pre-flight tests and radiation campaigns were performed before launch by the industrial partners of the mission. As part of this, a radiation dose distribution was predicted across the focal plane, upon which basis the laboratory irradiations were performed.[10] This prediction was made in 2006 using the predicted level of Solar activity at the time. Hardware and performance optimization strategies were devised, and the mission was expected to meet mission astrometry requirements for no longer than five years.

In order to keep track of Gaia's performance throughout its mission, routine operations are run which include several in-flight calibration activities. From analysis of some of this in-flight calibration data, it was found that the degradation of signal in the Gaia CCDs from radiation damage was much less than was initially expected from the pre-launch tests.[11,12] After more than six years in orbit, the increase of CTI has not differed significantly from the previously measured trend although that is likely to change given the onset of a new solar cycle in recent years.[13] Figure 1 illustrates the trailing charge CTI as measured by irradiated on-ground devices as the in-flight CTI from multiple CCDs at two different points in the mission, albeit at different periods between in-flight and on-ground. The details of these in-flight results are outlined in another study.[13] The on-ground CCD was irradiated at room-temperature at Gaia's predicted in-flight fluence levels with a safety margin added.

While the lower CTI levels are a positive outcome for the science objectives of the mission, it is important to understand, as best as possible, the reasons for this discrepancy. This is to make sure adequate and accurate testing can be performed in the future for other space missions and for confidence in the results of pre-flight tests. In the case of Gaia, a number of different hypotheses have been proposed to explain the difference in CTI between the in-flight and on-ground CCDs such as the in-flight straylight levels, the lower solar activity, and the irradiation environment.[12,13]

Analysing the CTI results directly can quantitatively tell us how much the CTI differs between in-flight and on-ground, as illustrated in Figure 1. To understand the CTI as accurately as possible however, it becomes important to try and model the charge data in order to understand the trap defect landscapes responsible for the CTI. These trap landscapes can then be used to infer details about the CTI and can be compared to other

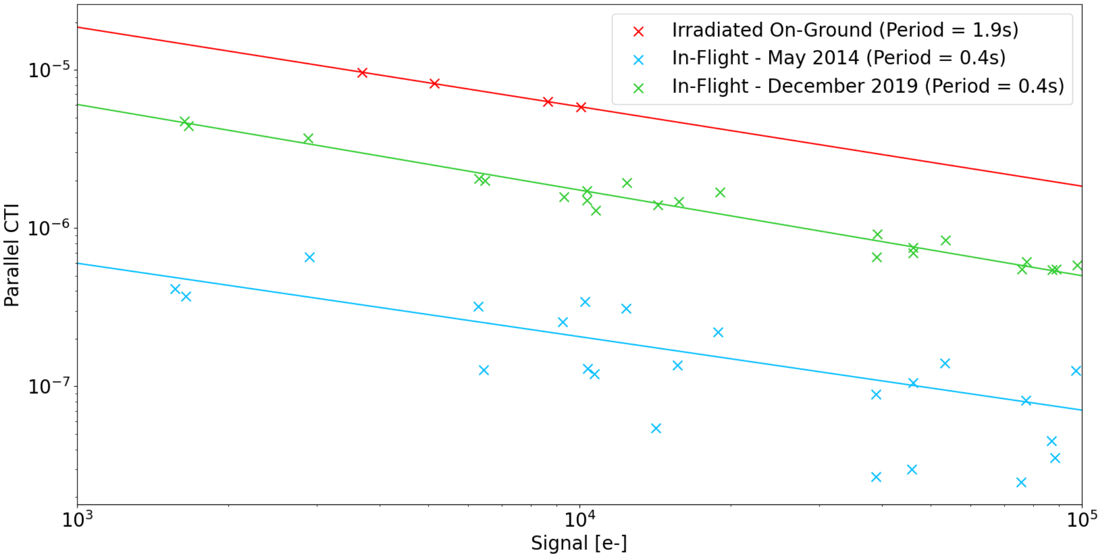


Figure 1: A comparison of the EPER CTI measurements from a number of in-flight devices at two different points in the mission and from an irradiated laboratory device. It is noted that the periods between the in-flight and on-ground data are different so the CTI differences should be taken as an approximation.

factors that affect CTI. In the ideal scenario, it would be possible to perform an analysis technique such as trap-pumping to directly measure the trap landscape,[14] which would allow for the level of radiation damage itself to be measured through the number of trap defects without the complications of straylight and other factors. This is not possible within the operating constraints of the mission so the next best step is to try and model the CTI to infer the trap defect landscapes. A number of different models have been developed to model CTI effects in irradiated CCD devices across multiple missions operating under different conditions, as discussed below.

4. MODELS AND SIMULATIONS

4.1 Charge Distortion Model

The Charge Distortion Model (CDM) was developed in the context of Gaia as a software correction technique of CTI effects. CDM was developed as a forward-modelling approach as opposed to a corrective approach to retain the noise properties of the data and to treat dispersed spectra and non-point source objects in the same way as single isolated stars. It was designed for speed over physical accuracy and while the model is based on physical Shockley-Read-Hall theory, it makes several simplifications to make sure it is computationally inexpensive. This includes treating electron trapping and de-trapping within each CCD column in a single step as opposed to treating the capture and emission of each electron separately. Some of the parameters used by CDM include the number of different trap defects as well as their corresponding emission time constants and trap densities. CDM was designed to work with a CTI-free image and an observed image; the model parameters would then be adjusted iteratively until a CTI-distorted predicted image is produced that best matches the observed image.[15]

4.2 Pyxel

Pyxel is a simulation toolkit developed collaboratively between the European Space Agency and the European Southern Observatory for end-to-end detection chain simulation. It was designed to simulate a variety of different detector effects, drawing on all the simulation models developed in the past for different space missions. The aim of Pyxel was for users to be able to test different detector effects at all levels from the pixel to the image level. Pyxel has several built-in CTI models, one of which being Gaia's CDM model.[16]

Pyxel was also developed with several different operating modes, based on the requirements of the user. One of these modes is a calibration mode which optimises a model or detector parameters to best-fit a user-defined target dataset. This was how CDM was originally designed to be run but with the bonus of built-in optimisation algorithms to find the best matching results.[16] Calibration mode requires input and target datasets, and parameters are found that can distort the input data to best match the target data.

4.3 C3TM

The Centre for Electronic Imaging (CEI) CCD Charge Transfer Model, or C3TM,[8] is another simulation model designed to simulate the physical processes and effects when transferring a signal through a radiation damaged CCD. It is computationally more expensive than CDM, but this is because it was designed to replicate physical effects in the CCD as accurately as possible. It uses electron density simulations developed in TCAD as an input which contain detailed information about the device such as the electrode layout and doping profiles. C3TM is a Monte Carlo model based on Shockley-Read-Hall theory and can operate on a sub-electrode level. It specifies several properties of trap defects such as their emission time constant, capture cross-sections and even their three-dimensional position in the pixel. This means the model can simulate different CCD clocking schemes like multi-level clocking and trap pumping which can be verified with experimental results.[8]

5. PYXEL CALIBRATION RESULTS

As a first step to modelling the data, Pyxel's calibration mode was used with CDM to find the best parameters that would model and describe the behaviour in the in-flight and on-ground data. For the in-flight data, the charge calibration data from May 2014 was taken as the input and the charge calibration data from December 2019 was taken as the target so the Pyxel results should represent the trap defects formed over five years of radiation damage accumulation. For the on-ground data, the irradiated on-ground charge calibration data was taken as the input and the target with the charge tails removed in the input data; the Pyxel results should represent the trap defects formed from the on-ground irradiations. The modelling was done in the parallel transfer direction so the results would be characteristic of the 982.8µs TDI clocking time.

From the Pyxel calibrations, it was found that three trap defects were sufficient to model the CTI in the in-flight and on-ground datasets. Using fewer than three traps resulted in lower quality fits while using more than three traps resulted in overfitting, where the same trap would be fitted twice. Table 1 details the Pyxel calibration results for the CDM trap defect parameters that best describe the on-ground charge calibration data while Table 2 details the same results but for the in-flight data. These results were obtained from a previous study that performed Pyxel calibrations with the Gaia data; the on-ground data is taken from a different irradiated CCD as compared to the previous study.[17]

Table 1: Pyxel best fit trap parameters for the on-ground calibration data

Trap No.	$\tau_e(s)$	Trap Density $(traps/cm^3)$
1	7.9×10^{-4}	1.4×10^{9}
2	1.4×10^{-2}	1.5×10^{9}
3	1.4×10^{-1}	5.7×10^{9}

When comparing the results of Table 1 and Table 2, it is noted while two of the fitted emission time constants of two trap defects are the same order of magnitude between each other, they are not entirely the same nor do they match the emission time constant values of any expected trap defects. This is because CDM does not simulate all the physical effects and the fitted traps are actually the best fits from a collection of multiple trap defects in the CCDs producing non-linear effects. Furthermore, the trap densities are likely not physically realistic either but best-fitting "effective" trap densities.[15,17]

Table 2: Pyxel best fit trap parameters for the in-flight calibration data

Trap No.	$\tau_e(s)$	Trap Density $(traps/cm^3)$
1	4.7×10^{-4}	6.9×10^8
2	3.6×10^{-3}	2.5×10^8
3	2.3×10^{-2}	4.2×10^8

These limitations were noted before and are likely to be due to the limitations of CDM. CDM was designed for computational speed and to model the data as accurately as possible. The results in Table 1 and Table 2 do indeed replicate the behaviour in the on-ground and in-flight data very accurately. However, for the objectives of getting a better understanding of the trap defect landscapes, the Pyxel and CDM results only reveal so much information and so other simulations need to be used, such as that of C3TM.[17]

6. CDM AND C3TM COMPARISONS

As discussed previously, while C3TM is computationally more expensive, it is able to accurately replicate more physical effects such as charge recapture. Due to the phenomenon of charge recapture, a charge tail from a single trap defect can be fitted with two different exponentials, illustrated clearly in Figure 5 of Skottfelt (2017).[8] This feature is loosely highlighted in Figure 2 where the charge tails from charge injections are plotted, as simulated in C3TM and CDM. The CDM charge tails are made using two of the fitted on-ground trap defects from Pyxel's calibration mode, as detailed in Table 1. The C3TM charge tail is made with a certain density of the trap defect known in the literature as the "unknown".[9]

It can be seen in Figure 2 that while the charge tails from CDM do not replicate the behaviour of the C3TM

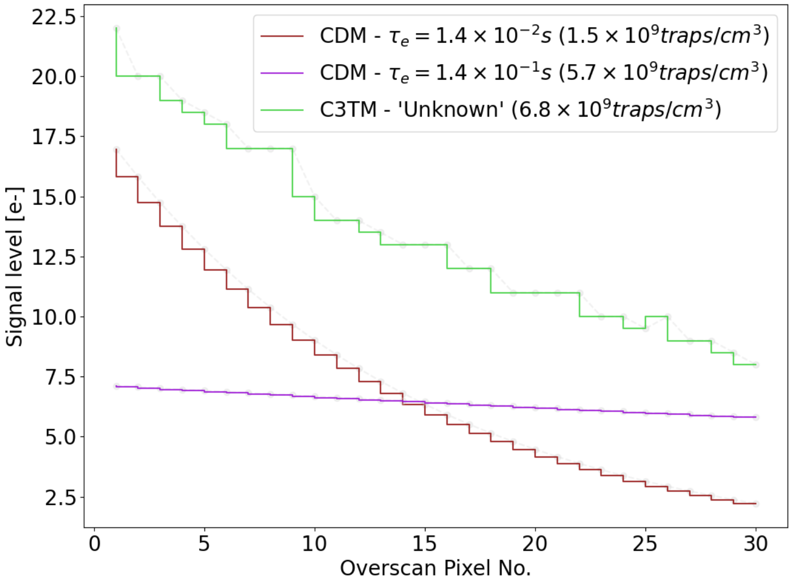


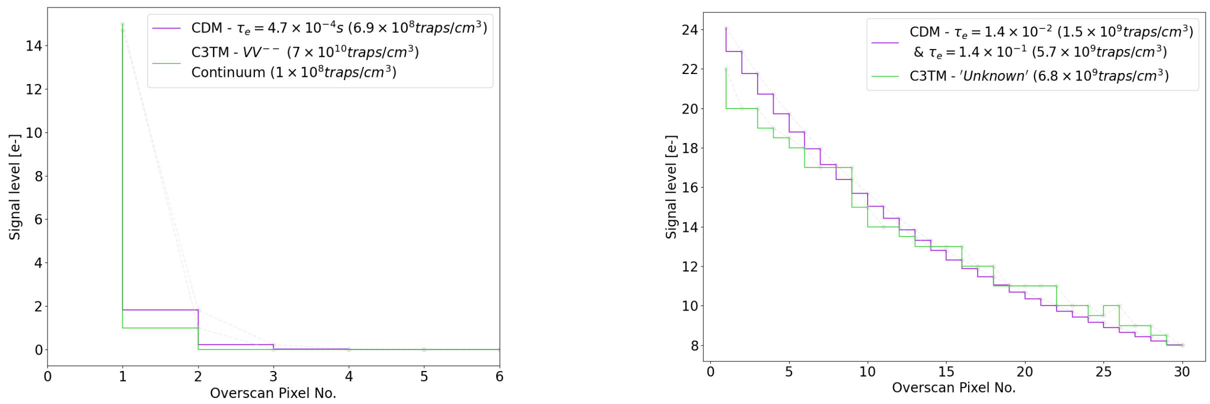
Figure 2: Charge tails following a 10,000-electron charge injection as simulated in C3TM and CDM. The CDM charge tails are made using the emission time constants and effective trap densities calculated with Pyxel's calibration of the on-ground data while the C3TM charge tail uses a given density of the "unknown" trap defect.

charge tail very well, they both replicate different parts of the C3TM charge tail reasonably well. This likely suggests that two of the traps fitted by Pyxel are actually manifestations of a single trap defect. While the CDM results from Pyxel may not be physically realistic, they accurately model real, physical effects. The approach taken next was to produce C3TM simulations of charge injections (CIs) and compare the charge tails to those produced by CDM. The C3TM charge tails and subsequent trap defect densities should likely be representative of the real trap defect landscapes within the Gaia CCDs.

The number of C3TM simulations that needed to be made was narrowed down by considering all the radiation induced trap defects detailed in the literature and comparing them to Gaia's operating parameters like clocking speed and temperature.[8,9] It was found that comparatively slower traps like the single vacancy and the E-centre do not produce any noticeable charge tails with respect to Gaia's operating parameters. The same is true for the A-centre which is too fast to produce any observable effects (although it has an impact in the serial direction). The radiation-induced trap defects that cause the greatest contribution to charge tails in the Gaia data were found to be the divacancy, the "unknown" and defects called the continuum. The continuum is a group of trap defects with a large spread of emission time constants that are found between the divacancy and "unknown" peaks in previous studies of trap defect landscapes.[18] The continuum has been noted to be produced in larger densities following a cryogenic irradiation as compared to room-temperature irradiations due to being physically stable at low temperatures and annealing at high temperatures; it is likely to be responsible for some of the differences in CTI between the in-flight and on-ground data.[19]

In order to model the most likely trap defect landscapes in the in-flight and on-ground datasets, C3TM CI simulations of the divacancy and "unknown" were generated and the charge tails were compared against corresponding charge tails from CDM CI simulations. A chi-squared fit was used to compare the charge tails against each other. The C3TM trap density where the charge tail best matched the CDM charge tail was taken as the "result" trap density. Once best-fit trap densities were found for the divacancy and the "unknown", different densities of continuum were added into the simulations to see if the chi-squared fits would improve. Figure 3a details the best-fit density of divacancy and continuum that matches one of the in-flight fitted CDM charge tails while Figure 3b details the best-fit density of "unknown" that best matches the cumulative effect of two of the on-ground fitted CDM trap defects.

A complexity should be noted about this procedure. While C3TM is adaptable for different CCDs, it requires semiconductor TCAD simulations as an input. At the time of this study, these simulations were only available for the CCDs of the Euclid mission and not the Gaia mission. While the C3TM parameters were adjusted to best



(a) (b)

Figure 3: (a) Charge tails trailing a 12,370-electron charge injection, as simulated using the fastest in-flight Pyxel calibrated defect from CDM and using a C3TM simulation of the best-fit trap densities. (b) Charge tails trailing a 10,000-electron charge injection, as simulated using two of the on-ground Pyxel calibrated trap defects in CDM and a C3TM simulation with the best-fit trap density.

match the Gaia CCD parameters as accurately as possible, there will likely be some discrepancies in the exact fitting. This means that the absolute trap densities may not be physically accurate however, the proportionate densities should be relatively accurate given that the trap parameters are correct.

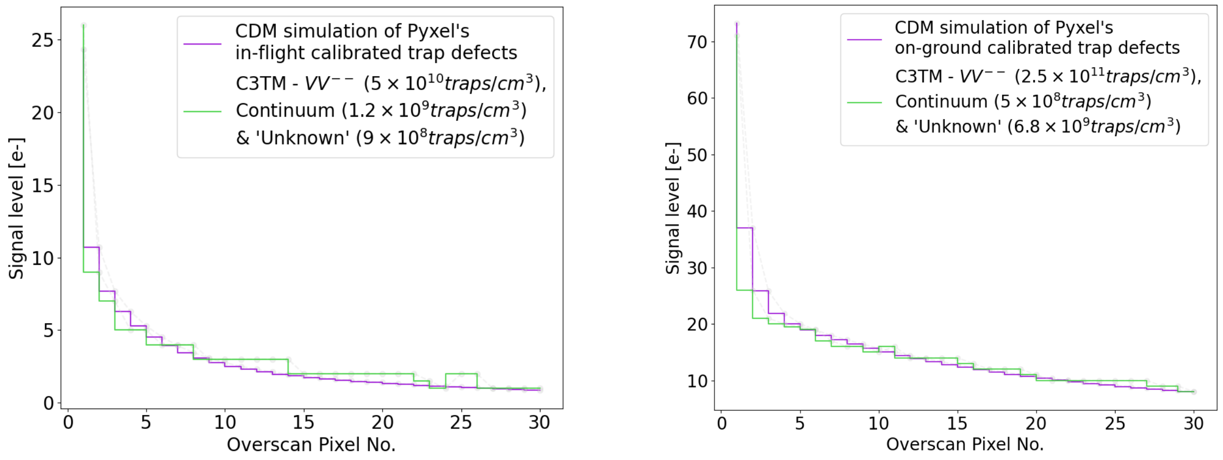
7. IN-FLIGHT AND ON-GROUND TRAP LANDSCAPES

Once the trap densities are found that best match the individual CDM simulations, they are all collectively simulated and compared against the cumulative effects of all the CDM parameters as given in Tables 1 and 2. When making the complete density fits, the C3TM densities were adjusted until the best chi-squared match was found between the complete CDM simulations and the C3TM simulations. Table 3 details the complete C3TM trap densities obtained for the in-flight and the on-ground data. As mentioned previously, these trap landscapes may not be exact but should be a very close approximation. These results are shown in Figures 4a and 4b; Figure 4a compares the charge tail between the CDM simulation of the Pyxel fitted parameters for the in-flight data against the charge tail from the C3TM simulation with the best matching trap densities; Figure 4b does the same but for the on-ground data.

Table 3: The best-fit C3TM trap densities that match the Pyxel fitted results for the in-flight and on-ground data

Trap Defects	In-flight modelled trap density ($traps/cm^3$)	On-ground modelled trap density ($traps/cm^3$)
VV^{--}	5×10^{10}	2.5×10^{11}
Continuum	1.2×10^{9}	5×10^{8}
"Unknown"	9×10^{8}	6.8×10^{9}

Interesting insights are revealed when comparing the in-flight and on-ground trap defect landscapes in Table 3. A larger density of continuum is obtained when modelling the in-flight data; this is likely reflective of the fact that in-flight CCDs experience radiation damage at cryogenic temperatures. As discussed previously from other studies, a greater proportion of continuum is obtained from cryogenic irradiations as opposed to room-temperature irradiations.[18, 19] This difference in continuum is most probably due to the different irradiation



(a) (b)

Figure 4: A comparison of the charge tails from a 10,000-electron charge injection between a CDM simulation using Pyxel's best fitted parameters and a C3TM simulation with the best fit trap densities for (a) the in-flight data and (b) the on-ground data.

conditions between in-flight and on-ground, given the fact that the on-ground irradiations were performed at room-temperature. In fact, it has been found that the continuum causes the largest proportionate amount of CTI in Gaia as compared to the other defects.

The on-ground data is modelled with larger densities of the "unknown" and the divacancy as compared to the in-flight data. These larger trap densities, and subsequent CTI contributions, are likely the primary reasons the on-ground data measures a higher CTI. The difference in density between the in-flight and on-ground results would suggest that the cumulative in-flight irradiation has not reached the levels used in the pre-flight on-ground irradiations. This suggestion lines up with the lower level of solar activity as compared to what was predicted pre-launch and is likely a big reason for the discrepancy between the in-flight and on-ground CTI.[12, 17]

8. CONCLUSIONS

The in-flight CTI of the Gaia devices has been measured to be much lower than what was expected from the on-ground tests. In order to get a greater understanding of why this has happened, charge calibration data from in-flight Gaia devices and on-ground irradiated devices has been modelled with different simulation models. Pyxel, using CDM as a charge transfer model, is able to obtain parameters that accurately model the physical effects of the data but does not provide realistic answers about the trap landscapes. In order to dig deeper, C3TM simulations were also generated and compared against CDM simulations of the Pyxel results to successfully obtain trap defect landscapes that describe the CTI behaviour in the in-flight and on-ground devices. From these trap landscapes, it has been found that while the cryogenic environment in space does lead to the greater production of a continuum of defects, the irradiation level in-flight has not reached the level of the on-ground irradiations, inferred from the differences in trap densities. This is suggested to be due to the lower-than-expected solar activity which seems to be responsible for the bulk of the difference between the in-flight and the on-ground CTI results. For future investigations, it would be useful to accurately model the radiation environment and get a measure of the dose obtained in-flight. This can be scaled with the results obtained in this study to get an assessment of the irradiation and corresponding CTI impact.

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