Chapter 4

Simulation of the HEX CdZnTe detector spectral response

The focus of this chapter is on simulation of the spectral response of the HEX CdZnTe detector. One of the nine detectors was chosen, characterized, and various experimental parameters were extracted. These were used as input to a Geant4 application developed to simulate the CdZnTe response, so as to reproduce the experimental results. This gives confidence in extraction of spectral parameters and in the methodology of the detector response simulation.

The primary detector of the HEX payload is composed of the compound semiconductor Cadmium-Zinc-Telluride (Cd\text{\textsubscript{1-x}}Zn\text{\textsubscript{x}}Te, x = 0.1). Compound semiconductors are characterized by a larger fraction of impurities and dislocations relative to silicon and germanium semiconductors, which are byproducts of the crystal growth technique. These impurities and dislocations in compound semiconductors act as charge carrier trapping sites. Loss of charge produced by incident ionizing radiation produces a visible distortion of the pulse height spectrum.

HEX is a spectroscopic instrument developed to measure the intensity of various γ-rays from the moon in the 30-270 keV range. In x-ray spectroscopy, the photon spectrum is measured in terms of counts as a function of channel numbers. This measured spectrum is related to the source spectrum by the response matrix, \( R(i,E) \)

\[
C(i) = \int_{0}^{E} f(E)R(i,E)dE
\]  

(4.1)

where

\( C(i) \) is the total number of counts measured in channel ‘i’, \( f(E) \) is the incident source
spectrum, which is to be determined, and \( R(i,E) \) is the instrumental response. It provides the probability that an incident photon of energy \( E \) will be detected in a channel ‘\( i \)’ of the ADC.

The instrumental response is a continuous function of energy, measured over a discrete number of channels. It can therefore be converted to a discrete response matrix \( R_{i,j} \) at discrete values of energy \( E_j \). In a response matrix, the incident energy \( E \) is redistributed across a set of channels. In order to determine the incident source and derive its parameters, a source model \( M(E) \) which best represents the characteristics of the incident photon source, is chosen and convolved with the instrument response to predict the observed spectrum corresponding to \( M(E) \). The predicted spectrum is then compared with the experimentally observed data; a ‘goodness of fit’ criteria is used to tune the parameters of the source model \( M(E) \), and finally the parameters that provides the optimum fit to the observed data is said to best represent the source.

The response matrix is the product of two components

\[
R_{i,j} = R_D(i,j) A(E_j)
\]  

(4.2)

where

\( R_D(i,j) \) is the spectral redistribution function (SRF), and is described as the probability that a photon of energy \( E_j \) is detected in a channel ‘\( i \)’; \( A(E_j) \) is the total effective area in cm\(^2\) which is the product of the detector geometric area and efficiency, \( \epsilon(E) \). Thus, the unit of the response matrix is cm\(^2\).

From the point of view of the HEX experiment it is necessary to construct the CZT detector response matrix. One of the initial steps involved towards this is to generate the SRF for all energies within the 30-270 keV range. This can in principle be achieved experimentally. However, practical constraints like unavailability of sources that cover the energy region of interest or infrastructure to conduct an extensive system calibration often prevents the experimental determination of the SRF across the full energy range.

Geant4 is an excellent tool for generation of detector SRF, because it takes into account all the physical processes of particle interaction with matter. It can be used to model the detector geometry as accurately as possible, with appropriate materials and dimensions, and irradiate with different radiation sources, either monoenergetic or any continuum.

This chapter focuses on the methodology for generation of the HEX primary detector SRF. First, experimentally measured spectral parameters are extracted from laboratory detector calibration data. These are then parameterized and used in an application to simulate the detector response.
The following section discusses the principle of pulse formation in semiconductor detectors, and will then we consider the factors that affect the shape of spectra produced by Cadmium-Zinc-Telluride detectors. This is important as understanding the structure of the measured spectra is essential in modeling the detector response.

### 4.1 Pulse Formation in Semiconductor Detectors

When a p-n junction is formed, majority carriers on either side of the junction diffuse into regions of lower concentration, forming a depletion region or junction with a contact potential which is due to a build up of space charge. This space charge arises from the immobile ions left behind when the majority charge carriers migrate.

When this junction is reverse biased (refer fig(4.1)), the flow of majority carriers across the junction is stopped. This is because, in addition to the contact potential, all the applied bias appears across the junction, creating a potential barrier that the diffusing electrons and holes cannot overcome. Thus, a high resistance is created for majority carriers across the junction. However, there is a small current across the junction due to the motion of minority carriers. Since application of a reverse bias increases the overall potential, there should be a corresponding increase in space charge and an extension of the depletion region into the p and n regions of the detector.

The total depletion region is therefore that region over which the space charge extends, which increases with the applied bias potential. Electron-hole pairs produced by ionizing radiation in the depletion region are swept towards their respective electrodes by this electric field. Semiconductors operated in the reverse bias mode are therefore used as radiation detectors.

Sensitivity requirements of radiation detectors demand interaction of incident particles in as large a volume as possible, so the greatest possible depletion depth is necessary.

The depletion width, $d'$, is given by the equation

$$d = \sqrt{\frac{2 \varepsilon V_0 \mu_0 \rho_{d'}}}{\mu}$$

(4.3)

where $\mu$ is the mobility of the majority carrier of the region with lower dopant concentration; $V_0$ is the applied voltage; $\epsilon$ is the dielectric constant; $\rho_{d'}$ is the resistivity of the depletion region in (\text{\Omega}\text{-cm}).
The depletion region has an inherent capacitance associated with it, which can be expressed in terms of capacitance per unit area

\[ C_a = \frac{\varepsilon}{d} = \sqrt{\frac{\varepsilon \varepsilon N}{2V_0}} \]  

(4.4)

where \( N \) is the dopant concentration of that side of the junction with the lower dopant concentration. Therefore, increasing the depletion width also decreases the capacitance, improving the noise quality of the system. A completely depleted detector is one in which the depletion region extends into the complete thickness of the detector, \( d \), and this happens for a particular value of bias voltage, \( V_d \). In this condition, the electric field \( \varepsilon \), in the depletion region is uniform and planar and is given by \( V_d/d \).

As discussed above, charge carrier pairs generated by ionizing radiation are swept to their respective electrodes by the electric field, and this occurs with a drift velocity

\[ \begin{align*}
    v_e &= \mu_e \varepsilon \\
    v_h &= \mu_h \varepsilon 
\end{align*} \]

(4.5)

These drifting charges give rise to induced charge on electrodes, which cause the bias voltage across the depletion region to reduce. A voltage appears across the load resistor of the external circuit which is equal to the amount by which depletion region voltage dropped. This voltage constitutes the basic signal, and it reaches a maximum when all the charges have been collected. It then returns to equilibrium depending on the time constant of the external circuit.

The amplitude of the voltage signal is proportional to the charge created by the ionizing radiation. Figure(4.1) shows a schematic of a semiconductor (SC) detector system. This schematic represents the dependence of the shape of the pulse on the location of interaction of the radiation within the depletion region.

For the sake of simplicity, it has been assumed that

- charges have been produced at a single position in the depletion region - there is no distribution of interaction positions
- the detector is completely depleted, with a high and uniform electric field
- there is no trapping of charges (this concept will be discussed in the next section)

In order to move from their place of generation, the charge carriers use the energy stored in the detector active volume (depletion region), given by \( \frac{1}{2}CV_0^2 \), where \( C \) is the
capacitance of the external circuit and \( V_0 \) is the bias voltage. If the point of generation of charge carriers is \( x_0 \), then the energy \( dE \), required to move total charge \( q_0 \) from there to some point \( x \) across a potential difference \( dV \) is

\[
\frac{dE}{dx} = -q_0 \frac{dV}{dx} = q_0 \varepsilon(x) = q_0 \frac{V_0}{d} \quad (4.6)
\]

where \( \varepsilon(x) \) is the electric field at \( x \). Integrating eqn(4.6) from \( x_0 \) to \( x \) gives the energy absorbed in moving the charge over this distance

\[
\Delta E = \frac{q_0 V_0}{d} (x - x_0) \quad (4.7)
\]

From this, the signal voltage across the load resistor \( R \) and the final collected charge are given by

\[
V_R = \Delta E = \frac{q_0}{C} (x - x_0)
\]

\[
Q = CV_R = \frac{q_0}{d} (x - x_0) \quad (4.8)
\]

As can be seen, the signal voltage and the final collected charge depend on the distance traveled by the charge carriers.

The charge collected as a function of time, \( Q(t) \) is dependent on the electron and hole charge collection times \( t_e \) and \( t_h \) respectively, which in turn depends on the point of interaction in the active volume. This in turn determines the electron drift distance \( x_e = v_e t_e \) and the hole drift distance \( x_h = v_h t_h \).

\[
Q(t) = \frac{q_0}{d} \times (\text{electron drift distance} + \text{hole drift distance}) \quad (4.9)
\]

Let the photon interact at a point distance ‘\( x \)’ from the anode. Let the electron-hole pairs be created at time \( t=0 \). Under the influence of the electric field the electrons drift a total distance \( x \) to the anode and the holes drift a total distance \( (d-x) \) to the cathode. When \( t<t_e \) and \( t<t_h \), the charge collection profile is given by

\[
Q(t) = q_0 \left( \frac{x_e}{d} + \frac{x_h}{d} \right)
\]

\[
= q_0 \left( \frac{v_e t}{d} + \frac{v_h t}{d} \right) \quad (4.10)
\]
Figure 4.1: Schematic of a semiconductor detector (adapted from [4a]) operated in the reverse bias condition. ‘d’ is the thickness of the detector which is completely depleted, and the direction of photon incidence is shown. The electron-hole pairs are formed in the direction of ‘d’ and ‘x’ is an example location of a photon interaction in the active volume (the region between the n+ and p+ contacts). The numbering in the active volume indicates five different positions where the photon can interact and produce charge carriers. Along side of the schematic are the shapes of the leading edges of the charge pulses formed due to motion of charge carriers from each of these locations to the electrodes. From this figure, the dependence of the pulse shape on the location of charge production is clearly visible.
Consider two cases

- when the interaction point is close to the anode: the electrons are collected faster than the holes, which will still be drifting
  
  For $t_e < t < t_h$

  \[ Q(t) = q_0 \left( \frac{x}{d} + \frac{v_h t}{d} \right) \]  

- when interaction point is close to the cathode: the holes are collected faster than the electrons, which will still be drifting
  
  For $t_h < t < t_e$

  \[ Q(t) = q_0 \left( \frac{v_e t}{d} + \frac{(d - x)}{d} \right) \]  

In addition to the shape of the leading edge of the charge pulse, the amplitude of the pulse is also affected by the position of interaction of the photon in the detector. This will be discussed in section 4.3.

### 4.2 CdZnTe Radiation Detectors

Silicon (Si, Z=14) and Germanium (Ge, Z=32) are the most widely used SC materials for radiation detectors. They provide good energy resolution at x-ray and γ-ray energies among all radiation detectors; this is due to their small band gaps (1.12 eV and 0.7 eV for Si and Ge, respectively). They are also excellent for timing studies due to their fast time response. The reasons that these detectors and scintillators are not good choices for hard x-ray spectroscopy in deep space missions are summarized in section 1.1.2.

It is desirable to have a radiation detector with energy resolution better than that of scintillators at hard x-ray energies, without the need for cryogenic cooling. This is where wide band-gap SCs come in—these are basically compound SCs, which are alloys between elements from the II, III, IV, V and VI groups of the periodic table. Typical SC materials are shown in table(4.1) Compound SC have band gaps wide enough for room temperature operation. At x-ray energies, line broadening is dominated by leakage current. This can be minimized by employing Peltier coolers or by passive cooling, using radiative plates.

Cd$_{1-x}$Zn$_x$Te (Cadmium-Zinc-Telluride or CZT) is a ternary compound of CdTe and ZnTe, where x is the blending fraction of ZnTe in CdTe. Alloying Zn in CdTe, another room temperature γ-ray detector, allows “stretching” of the band gap. Varying x from...
Table 4.1: List of Semiconductor Materials from [1d]

<table>
<thead>
<tr>
<th>Standard SC</th>
<th>Si, Ge</th>
</tr>
</thead>
<tbody>
<tr>
<td>II-VI compound</td>
<td>CdS, CdSe, CdTe, ZnS, ZnSe, ZnTe, Hg_{1-x}Cd_xTe, Cd_{1-x}Zn_xTe</td>
</tr>
<tr>
<td>III-V compound</td>
<td>GaP, GaAs, GaSb, InP, InAs, InSb</td>
</tr>
<tr>
<td>IV-VI compound</td>
<td>PbS, PbSe, PbTe, Pb_{1-x}Sn_xTe, Pb_{1-x}Sn_xSe</td>
</tr>
<tr>
<td>IV-IV compound</td>
<td>SiC, Si_{1-x}Ge_x</td>
</tr>
<tr>
<td>V-VI compound</td>
<td>Bi_{2}Te_{3}</td>
</tr>
<tr>
<td>Chalcopyrite</td>
<td>AgGaS, AgGaSe_{2}, CuInS_{2}, CuInSe_{2}, ZnGeP_{2}, CdGeP_{2}</td>
</tr>
</tbody>
</table>

0.04 to 0.2, the band gap can be varied from 1.53 eV to 1.64 eV. The increased band gap increases the resistivity ($10^9$ ohm-cm), lowers the leakage current, and hence allows operation at higher temperatures. Resistivities of CZT detectors are one to two orders of magnitude higher than that of CdTe detectors.

CZT is a very attractive SC detector material for hard x-ray/soft γ-ray astronomy and

- has a higher stopping power than Si, as it is three times more dense
- has a greater photoelectric to Compton cross-section ratio that either Si or Ge because its effective atomic number, $Z_{eff}$ is 50, compared to $Z$ of 32 for Ge and $Z$ of 14 for Si
- facilitates operation at higher temperatures, providing a compact, energy-efficient detection system

CZT detectors can be fabricated as planar detectors with monolithic electrodes, or with pixellated or cross-strip read-out which can be used for position sensing. CZT detectors are being used on the Burst Alert Telescope (BAT) on the SWIFT mission [2d]. The Energetic X-ray Imaging Survey Telescope (EXIST) [3d] plans to use CZT detectors along with a coded mask aperture, for imaging in the 5-600 keV energy region. The Atmosphere-Space Interaction Monitor (ASIM) [4d] will be mounted on the International Space Station (ISS) to study the impact of space weather on our atmosphere, and will include a Modular X and Gamma-ray Sensor (MXGS) that uses CZT detectors in the 7-500 keV energy region. CZT and CdTe detectors have wide applications in medicine and a comprehensive review can be found in [5d].

The disadvantage of CZT detectors, and compound detectors in general are their poor charge carrier transport properties; in CZT, the mobility $\mu_e$ of electrons is an order of magnitude higher than that of holes. Due to the crystal growth techniques, stresses, dislocations and impurities populate the band structure, leading to reduced lifetime of holes $\tau_h$ in the crystal, compared to electrons. Carrier lifetime defines the time before
a carrier is trapped in the crystal lattice due to recombination at impurity or dislocation sites. This will be discussed in detail in the next section.

Leakage currents are reduced when the resistivity of the material is high, which is the case when the purity of the material improves. There are techniques employed to create high purity materials, but there will still be some trace impurities left behind in the material - this results in the material being either slightly n-type (represented by the symbol ‘ν’) or slightly p-type (represented by the symbol ‘π’), depending on the predominance of the residual donor-type or acceptor-type impurities. Materials are also compensated, which means that residual impurities are balanced out by doping the purified material with donors of the opposite type of the impurities. The material still ends up being either ν or π, because of the difficulty to precisely balance out the concentration.

It is desirable to use fully depleted SC as radiation detectors. When a heavily doped material (designated as \( p^+ \) and \( n^+ \)) is placed in contact with a lightly doped or intrinsic material of the opposite type, the depletion width extends into the lightly doped region. This happens in order to balance the charge on either side of the junction. On the heavily doped side, the depletion width is very thin.

When a purified or compensated material is placed between thin layers of \( n^+ \) and \( p^+ \), one of the contacts is a rectifying contact while the other one is a blocking or non-injecting contact. This depends on whether the material in between, is ν or π. A rectifying contact is one that forms a depletion region at the contact, and blocking contact prevents injection of majority carriers into the SC. In the reverse bias condition, the positive terminal is always connected to \( n^+ \) and the negative to \( p^+ \). Contacts can be also be made between metals and SC ; metal-SC contacts (MSC). These can be either of blocking (Schottky) kind or ohmic kind.

A Schottky MSC has current-voltage (I-V) characteristics similar to that of a p-n junction, while for an ohmic MSC, the I-V characteristics are linear, following Ohm’s law. The difference between the two is in the barrier height in the SC for electrons - it is narrower for ohmic contacts than for Schottky contacts. Due to the lower barrier height in ohmic contact, there is an easier flow of electrons from the SC to the metal; this constitutes an additional noise factor in addition to the thermal motion of electrons, which is present in Schottky contacts as well. Therefore, the leakage currents measured in devices with ohmic contacts are an order of magnitude higher than those measured in devices with Schottky contacts.

Tests have been performed on CZT detectors to study the dependence of resistivity and hence leakage currents on the type of contacts used [8d]. Standard IMARAD CZT detectors [6d] (from Orbotech) use Indium-Indium ohmic contacts, which showed an
order of magnitude higher leakage current compared to CZT detectors with blocking contacts.

Radiation damage in SC affect the charge lifetime, charge collection efficiency and leakage currents. Displacement of atoms from the crystal lattice to interstitials result in the formation of charge traps. This causes incomplete charge collection, and hence degradation in resolution. Resolution also worsens due to increasing leakage current. Incomplete charge collection also affects the gain of detector, which corresponds to shift of the peak channel.

The CZT modules used for the HEX instrument have been procured from Orbotech Medical Solutions, Israel [6d], grown by the modified Horizontal Bridgman technique. The specifications of these modules are listed in table (4.2)

<table>
<thead>
<tr>
<th>Property</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>5.85 g cm$^{-3}$</td>
</tr>
<tr>
<td>Bulk resistivity</td>
<td>$3.8 \times 10^9$ ohm-cm</td>
</tr>
<tr>
<td>Mean Zinc content</td>
<td>9-11%</td>
</tr>
<tr>
<td>Electron-hole production energy</td>
<td>4.43 eV</td>
</tr>
<tr>
<td>Electrode type</td>
<td>Ohmic</td>
</tr>
<tr>
<td>Electrode material</td>
<td>Indium</td>
</tr>
<tr>
<td>CZT material type</td>
<td>n-type</td>
</tr>
<tr>
<td>Cathode</td>
<td>Monolithic</td>
</tr>
<tr>
<td>Anode</td>
<td>Pixellated</td>
</tr>
<tr>
<td>Number of pixels</td>
<td>256</td>
</tr>
<tr>
<td>Anode pad size</td>
<td>1.86 mm $\times$ 1.86 mm</td>
</tr>
<tr>
<td>Pixel pitch</td>
<td>2.46 mm</td>
</tr>
<tr>
<td>Read out</td>
<td>XAIM 3.2 ASICS, IDEAS, Norway</td>
</tr>
<tr>
<td>Number of channels per ASIC</td>
<td>128</td>
</tr>
<tr>
<td>Number of ASICS per module</td>
<td>Two</td>
</tr>
<tr>
<td>Expected energy resolution (25°C)</td>
<td>5% at 122.1 keV</td>
</tr>
</tbody>
</table>

| Table 4.2: Specifications of the CZT modules procured from Orbotech Imaging for the HEX instrument |

### 4.3 Charge trapping and Pulse Amplitude

Recent compound SC growth techniques are still not able to completely eliminate crystal non-uniformities, defects, and impurities. These defects in the crystal lattice can act as traps for charge carriers as they drift along electric field lines. Traps are energy levels or centers in the band gap of the crystal that rapidly capture charge carriers and then release them at a much slower rate. Impurities in the SC, like positively charged donor ions in n-type materials and negatively charged acceptor ions in p-type materials have
their energy levels in the SC band gap and act as traps. If charges are trapped in the lattice while they drift towards their respective electrodes, they will not be able to contribute to the measured current signal. Therefore, the signal measured in the presence of traps have a smaller amplitude than signals measured in the absence of traps.

In the absence of an applied electric field, an excess charge created in a SC due to external processes like thermal energy or ionizing radiation causes the equilibrium of the system to get disturbed. The system reverts back to the equilibrium condition by the process of recombination. The simplest way that electrons and holes can recombine is via band-to-band recombination, in which an electron in the conduction band fills a hole in the valence band. Charge carrier traps, as discussed above, have energy levels in the SC band gap and are called recombination-generation centres (RGC). Recombination of an electron or hole with a charge trap is called trapping and can be defined as

- **electron trapping** - transfer of an electron from the conduction band to the RGC
- **hole trapping** - transfer of an electron from RGC to the valence band

This is illustrated in the fig(4.2).

![Figure 4.2: This is a schematic representing charge trapping. The shaded regions are the conduction and valence bands, while the dashed lines in the band gap are the recombination-generation centres (RGCs). The transfer of an electron from the conduction band to the RGC represents electron trapping, while the transfer of an electron from the RGC to the valence band is hole trapping.](image)

When the thermal equilibrium of a SC is disturbed, the rate of recombination should increase to bring the system back to equilibrium. In the case of electrons and holes, the capture rates are proportional to
the concentration of traps or R-G centres, $N_t$

- the concentration of carriers at thermal equilibrium

- the probability that a trap site is occupied by an electron, $f_t$, which is given by Fermi-Dirac statistics (pertinent to hole trapping)

$N_t$ is larger in compound SC like CZT compared to Si and Ge. In an n-type compound SC, the Fermi level lies close to the bottom of the conduction band, which means that all trap levels below it have an electron occupancy of 1; the event of a hole encountering such a R-G site always ensures its capture. For p-types, the concentration of holes is large at thermal equilibrium, and so the capture rate is higher compared to that of electrons. This means that the lifetime of a hole, or the average time before a hole encounters a RGC, in either n-type or p-type material, is short. This fact coupled with the low intrinsic mobility of the holes compared to the electrons ensures that holes have poorer charge transport properties than electrons.

For a charge carrier, the product of the mobility $\mu$, the lifetime $\tau$ and the electric field strength $\varepsilon$ is $\lambda$, the trapping length of the carrier and is the distance that the carrier can travel in the detector under the influence of $\varepsilon$, before it is trapped. Typically, the electron and hole mobility-lifetime products, ($\mu\tau)_e$ and ($\mu\tau)_h$ are $10^{-3}\text{ cm}^2\text{V}^{-1}$ and $10^{-5}\text{cm}^2\text{V}^{-1}$ respectively for CZT detectors. For a bias voltage of -500 V and detector thickness of 0.5 cm, the electric field is $1000\text{ Vcm}^{-1}$. Assuming that the field within the detector is uniform, one can compute $\lambda_e$ as 1 cm and $\lambda_h$ as 0.01 cm. If the distance ‘x’ that a charge carrier has to travel to reach its electrode is greater than its $\lambda$, the probability that this charge is lost through trapping is higher than for a carrier whose $\lambda$ is greater than x. From the above numbers, it is obvious that the holes have a higher probability of getting trapped than electrons.

The poor transport properties of holes demand illumination from the cathode side of the detector; holes generated near the cathode by low energy incident radiation do not suffer the kind of trapping that holes generated by more penetrating radiation do. High energy x-rays and $\gamma$-rays are more penetrating and interact through out the detector active volume. Holes generated near the anode have to traverse a path that is longer than their trapping length and hence are lost and cannot contribute to the total charge collected.

From eqn(4.9), it can be seen that the total induced charge is dependent on the distance traveled by the electrons and holes. In the absence of charge trapping, the shape of the charge pulse is dependent on the distance traveled. However, the presence of traps also affects the amplitude of the charge pulse, because once a charge carrier has been
trapped in an RGC, it is no longer mobile and does not contribute to the induced charge. So the signal collected will have an amplitude that is always less than what it should have been in the absence of charge trapping. The Hecht equation [24d]

\[ \eta = \frac{\lambda_e}{d} \left( 1 - e^{-\frac{(d-x)}{\lambda_e}} \right) + \frac{\lambda_h}{d} \left( 1 - e^{-\frac{x}{\lambda_h}} \right) \]  

(4.13)
gives the charge collection efficiency (CCE), \( \eta \) which is the ratio of the charge induced at the electrodes to the total charge created at the site of radiation interaction in the detector, and it shows the dependence of interaction position on the amplitude of the signal pulse. In eqn(4.13), \( x \) is the distance of the interaction position from the cathode, and \( d \) is the depletion width or the active thickness of the CZT detector. From this equation it can be seen that going for thinner detectors improves \( \eta \). Also, increasing the bias voltage increases the trapping lengths thus improving \( \eta \). Hole trapping causes signal pulses due to monoenergetic radiation, to have varying amplitudes, and these manifest themselves in pulse height spectra as “tails” at the low energy side of the Gaussian photopeak. The number of counts in the photopeak is larger for the same photon energy in the absence of trapping than otherwise. Trapping of electrons however, results in gain shifts or shifts in the photopeak position in the pulse height spectra.

The spectra of high energy photons measured by CZT detectors show more prominent hole tails than low energy photons that interact near the cathode. This leads to lower spectral peak sensitivity, which is defined as the ratio of the counts under the photopeak to the total counts under the spectrum. When a radiation source consisting of multiple photon energies are measured by CZT detectors, the sensitivity of low energy peaks are lost, because of the increased low energy continuum, caused due to overlap of hole tails of higher energy spectral lines. So, loss of line-to-continuum sensitivity is the major effect of hole trapping in CZT detectors.

Hole tailing is important in applications where the distance that the carriers have to travel is larger than the trapping length. It depends on the energy of the photons that are being measured. The carrier lifetimes vary within a single detector, so careful calibration of the detector and subsequent extraction of the mobility-lifetime products for both electrons and holes, \( (\mu \tau)_{e,h} \) is an important part of detector characterization.

This chapter focuses on the simulation of the HEX CZT detector response using Geant4. Experimental determination of \( (\mu \tau)_{e,h} \) products is an essential part in the modeling of CZT spectral response, along with experimental measurements of variation spectral parameters with energy. This experimental characterization is discussed in the next section.


4.4 Laboratory Tests on a single CZT module

The nine CZT detectors used in HEX were characterized at the Physical Research Laboratory (PRL) Ahmedabad in a hot-cold chamber. The details of the experimental set up and experimental methodology can be found in [25d]. The radioactive sources $^{241}$Am and $^{57}$Co were placed at appropriate distances from the test set up so as to enable uniform pixel illumination. The chamber temperature was varied from $-20^\circ\text{C}$ to $25^\circ\text{C}$ in steps of $5^\circ\text{C}$. At each temperature, spectroscopic measurements were made at three different operating bias values, -500 V, -600 V and -700 V. For the present work, only data measured by one of the flight detectors B11290, was analyzed for extraction of $\mu\tau$ products and spectral parameters, with the assumption that the overall response of other detectors were not significantly different.

4.4.1 Extraction of Mobility-Lifetime products

The method of extraction of charge carrier mobility-lifetime ($\mu\tau$) products has been adapted from [26d]. Here, the pulse height spectra recorded by the detector at different bias voltages are fit simultaneously with a model that take into account a Gaussian photopeak and a low energy exponential tail. This exponential tail follows from eqn(4.13). So in effect, the pulse height spectrum is modeled and this model is then fit to the experimental data to extract the ($\mu\tau$)$_{e,h}$ products.

The spectra due to 122.1 keV photons from the $^{57}$Co source were used to extract the ($\mu\tau$)$_{e,h}$ values, as photons of this energy interact throughout the active volume of the detector and its spectral shape best represents the charge carrier transport properties.

Raw data were reduced using specifically written PERL scripts for further analysis using Sherpa [27d] in CIAO [28d]. CIAO (Chandra Interactive Analysis of Observations) is a flexible, multi-dimensional software designed for the analysis of data from Chandra X-ray Observatory. The design of CIAO is mission independent - it can be used to analyze data from any another mission or even laboratory data. All CIAO tools read and write in several formats, from ASCII text to FITS images and tables. Sherpa is the modeling and fitting tool of CIAO, which fits models to N-dimensional data. In addition to Sherpa’s built-in models, user-defined models can be constructed and registered with Sherpa, and used in same manner as the built-in models. The scripting language S-Lang [29d] has been embedded in CIAO, and is used to extend the functionality of Sherpa. S-Lang is an array based language, featuring conditional and looping syntax, global and local variables, user-defined structures and functions, and to a lesser extent, pointers.
The model to fit the $^{57}$Co data was written in S-Lang. The $^{57}$Co pulse height spectrum is modeled in S-Lang as follows:

1. The detector was divided into a number of thin slices.

2. Using the attenuation coefficient for the photon energy under study, the interaction probability $dI(x)$ was calculated for each depth $dx$. The total number of counts under the spectral region of interest is then multiplied by the interaction probability at each depth to obtain the counts detected at that depth.

3. Using the Hecht equation and $Ch_{max}$ (the channel number at which the Hecht equation is equal to unity), the pulse amplitude at each depth was computed. This was repeated for each operating voltage.

4. These pulse amplitudes are then convolved with a Gaussian distribution which represents the broadening due to Fano statistics and electronics noise.

5. The counts at each depth and the pulse height at each depth now give the model spectra for each operating voltage.

This model is compiled and executed in a Sherpa command batch script.

For a particular temperature, the $^{57}$Co data measured at one of the bias voltages, is split by a specifically written PERL script into 256 files, each file corresponding to one pixel. This is repeated for each of the other two bias voltages, resulting in a total of 768 data files for that temperature. So, for one temperature, a pixel of the detector will have three files attached to it, each file corresponding to a high voltage value.

The spectral fitting with the model is done pixel-wise. A Sherpa batch file reads in the three spectral data files corresponding to one pixel, and then compiles and registers the model before fitting the data.

The model consists of eighteen parameters, as each bias voltage has six parameters attached to it; $(\mu \tau)_e$, $(\mu \tau)_h$, spectral width parameter $\sigma$, electric field value, $Ch_{max}$, and the total number of counts within the region of interest of the spectrum used for the fitting. Out of these eighteen parameters, the electric field values are frozen, and the six $(\mu \tau)_{e,h}$ values are linked together as their values are dependent on the material properties. $Ch_{max}$ is that channel which corresponds to complete charge collection, in the absence of trapping. It is proportional to the total charge generated by the incident photon at the interaction site. It is independent of the applied electrical field, and so, in order to eliminate the effects of the electric field, data measured at three different bias voltages are fit simultaneously. Therefore, the three $Ch_{max}$ values are also linked. This brings the number of free parameters to nine, whose values are obtained from the fit.
The initial guess values of the parameters are supplied to the fitting algorithm, and the three data files are fit simultaneously with the model, till the best fit is arrived at, for this pixel. The same is done for all the other pixels.

This process is repeated for all the temperatures in the range over which the measurements were taken. Only those pixels that had clean spectra, i.e. spectra with well resolved photopeaks, were chosen for the analysis.

The fig(4.3) and fig(4.4) show the distribution of the \((\mu\tau)_e\) and \((\mu\tau)_h\) products respectively, over all clean pixels, for each temperature. These distributions were constructed by binning these values as a function of pixel number, i.e. by finding the frequency distribution of \((\mu\tau)_e\) and \((\mu\tau)_h\) products as a function of CZT pixel. This is repeated for each temperature.

The \((\mu\tau)_e\) distribution shows a bipolar trend for all temperatures. Averaging over temperature, about 80% of the pixels used in each distribution, fall in the larger peak. This bipolar trend indicates that the \((\mu\tau)_e\) values of some pixels are overestimated, that is, showing a smaller value than majority of these pixels. These pixels with smaller values of \((\mu\tau)_e\) could be the edge pixels of the detector module, as evidenced by studies in [31d] and references within. In order to verify this with respect to the HEX CZT, one has to map these pixels onto the CZT pixel map supplied by the manufacturer to see where these are located with respect to the crystal, i.e. whether they are edge pixels or inner pixels, or if they are randomly distributed over the crystal.

The \((\mu\tau)_h\) distribution on the other hand shows more deviation between pixels, for each temperature. The bi-polarity, if it exists as in the case of \((\mu\tau)_e\), would have been smeared out by this large deviation. Slight evidence of this bi-polarity can be seen for some temperatures. For the purpose of studying the variation of the \((\mu\tau)_{e,h}\) as a function of temperature, the data were averaged over all pixels. This was done for each temperature by taking the arithmetic mean over the pixels; this was used instead of Gaussian determination of mean because it was required to make use of data of all the pixels. The pixel averaged values are designated as \((\mu\tau)_{e,avg}\) and \((\mu\tau)_{h,avg}\).

Figure(4.5) shows the variation of \((\mu\tau)_{e,avg}\) and \((\mu\tau)_{h,avg}\) values with temperature. It can be seen that \((\mu\tau)_{e,avg}\) and \((\mu\tau)_{h,avg}\) vary linearly with temperature, with \((\mu\tau)_{e,avg}\) flatter than \((\mu\tau)_{h,avg}\). Linear fits to the data show that for every 5°C variation with temperature, \((\mu\tau)_{e,avg}\) varies by 0.7% while \((\mu\tau)_{h,avg}\) varies by 2.3%. The larger variation seen for \((\mu\tau)_{h,avg}\) is due to the inherent spread of the \((\mu\tau)_h\) values seen in fig(4.4).

Before one studies the significance of this variation of the charge carrier \((\mu\tau)_{e,h}\) with temperature, one must first understand the significance of these parameters on the shape of the pulse height spectrum. \((\mu\tau)_e\) defines the location of the peak or maximum value
Figure 4.3: Distribution of $(\mu\tau)_e$ over all pixels, for each temperature.
Figure 4.4: Distribution of $(\mu\tau)_h$ over all pixels, for each temperature.
of pulse height that is measured at a particular operating voltage. $(\mu \tau)_h$ defines the amount of tailing observed in a spectrum for a particular value of electric field and $(\mu \tau)_e$. For low values of $(\mu \tau)_h$, the counts under the photopeak or the **photopeak area** is less compared to high $(\mu \tau)_h$ values.

Using eqn(4.13) one can study the variation of $\eta$ over the detector thickness for different values of $(\mu \tau)_e$, $(\mu \tau)_h$, and electric field $\varepsilon$. One can define a “photosensitive” region of the detector as that depth of the detector which contributes to the photopeak of the spectrum. In order to define this, the benchmark for defining this region has been chosen to be that depth over which the $\eta$ varies from 100% to 70%. All subsequent $\eta$ calculations have been performed for the case of x-ray illumination from the cathode side.

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**Figure 4.5:** Pixel averaged $(\mu \tau)_e$ and $(\mu \tau)_h$ plotted as a function of temperature. The horizontal green lines in each plot are the $2\sigma$ limits.
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Figure 4.6: Charge collection efficiency (CCE) $\eta$, plotted as a function of interaction depth for an operating bias of 530 V, at a temperature of 0°C. $\eta$ was calculated using 3 different values of $(\mu \tau)_h$, as indicated, and the pixel averaged $(\mu \tau)_e$ value for 0°C. The x-axis represents the depth of the detector, from the cathode side. 0 cm indicates the cathode, and 0.5 cm indicates the anode.

Consider fig(4.6); it shows the variation of $\eta$ for different values of $(\mu \tau)_h$ at 0°C, computed using the eqn(4.13) - the electric field is calculated for 530 V (which is the CZT in-orbit operating bias voltage), and the $(\mu \tau)_e$ value used is the pixel averaged value. As can be seen, $\eta$ falls off faster for the lowest value of $(\mu \tau)_h$, compared to the slow fall for the highest value. In terms of the earlier definition for the photosensitive region,

- only 27% of the total detector depth contributes to the photopeak for the lowest $(\mu \tau)_h$ value; this means that for N photons of energy E that interact throughout the detector, 73% of the events fall under the low energy tail
- 86% of the total detector depth contributes to the photopeak for the highest $(\mu \tau)_h$ value; this means that for N photons of energy E that interact throughout the detector, 14% of the events fall under the low energy tail
- for the intermediate value of $(\mu \tau)_h$, the photosensitive region is 60% of the total detector depth; this means that for N photons of energy E that interact throughout the detector, 40% of the events fall under the low energy tail

This indicates the significance of $(\mu \tau)_h$ on the tailing observed in the pulse height spectra; lower the $(\mu \tau)_h$ value, larger will be the fraction of photopeak counts “lost” in the tail compared to that for higher $(\mu \tau)_h$ values.
Therefore, as seen in fig(4.5), the variation of \((\mu \tau)_{e,h}\) with temperature will be reflected in the shape of the measured pulse height spectrum.

Figure(4.7) illustrates the effect of increasing the bias voltage on the photopake efficiency. The temperature averaged values of \((\mu \tau)_{e,h}\) from fig(4.5) were used in eqn(4.13) to calculate \(\eta\) for 530 V, 600 V, and 700 V. There is a visible difference in \(\eta\) as seen in the figure, which corresponds to a difference of 12% in sensitive volume between the highest and lowest operating voltage value.

![Figure 4.7: Charge collection efficiency (CCE) \(\eta\), plotted as a function of operating voltage using the temperature averaged values of \((\mu \tau)_{e,h}\). The x-axis is along the depth of the detector, from the cathode side. 0 cm indicates the cathode, and 0.5 cm indicates the anode.](image)

The CCE also depends on the energy of the incident photon, which determines the distribution of photon interaction sites within the detector. In fig(4.8), 0 cm indicates the cathode and 0.5 cm indicates the anode for a 0.5 cm thick detector. The green dots in each plot is the interaction site or **depth of interaction (DOI)** of the incident photon in the detector. For the purpose of this calculation, photons of energy 30 keV and 122 keV were considered. The DOI for each energy in the CZT were extracted using Monte Carlo simulations. A simple simulation application was developed for a CZT detector modeled with appropriate materials; \(\gamma\)-ray photons where made to illuminate the region of the crystal which was designated as the cathode. For each incident photon energy, the DOI in centimeters was extracted and written into an output file. For each energy, the DOI were inserted into eqn(4.13) to compute \(\eta\). The \(\eta\) for each energy is indicated by the red points in fig(4.8). The \((\mu \tau)_{e,h}\) values used in the calculation of \(\eta\) were the
temperature-averaged values as shown in fig(4.5) and the operating voltage used was 530 V.

From the plots it can be seen that all the 30 keV interactions contribute to the photopeak (defined by the photosensitive region discussed above), while only 60% of the 122 keV interactions in the detector contribute to the photopeak. This is because of the difference in DOI distribution between the two energies; for 30 keV, the DOI distribution is tightly bunched near the cathode (corresponding to depth 0 cm), while for 122 keV, the DOI distribution is more or less spread over the detector volume. This indicates that the 30 keV spectral peak will show insignificant tailing compared to the 122 keV peak.

![Diagram](image)

**Figure 4.8:** Variation of charge collection efficiency (CCE) \( \eta \), with incident photon energy. The x-axis represents the depth of the detector, from the cathode side. 0 cm indicates the cathode, and 0.5 cm indicates the anode. The top plot shows the variation of \( \eta \) with interaction depth in the detector for 30 keV. The green squares represent the depth of interaction (DOI) of each of the incident 30 keV photons within the detector, and the red points represent the \( \eta \) value at that DOI. The same applies to the bottom plot which shows the variation of \( \eta \) with DOI in the detector for 122 keV.

To summarize

- Knowledge of the detector charge transport properties is essential for accurate modeling of the CZT detector response.
- \( (\mu \tau)_e \) determines the location of the maximum pulse height amplitude.
• \((\mu \tau)_h\) determines the low energy tailing in the spectrum.

• Photopeak efficiency (ratio of photopeak area to area under spectrum) improves with larger values of \((\mu \tau)_h\).

• Lower energy photons exhibit little or no tailing in their spectra, while it is enhanced for higher energy photons.

In order to complete the modeling of the detector response, one must extract spectral parameters from the experimental data and study their variation with energy and temperature.

### 4.4.2 Extraction of Spectral Parameters

The spectral parameters for CZT module B11290 were extracted by analyzing the data measured by the detector at -500 V, for different temperatures. This voltage value was chosen because it is closest to the voltage that will be used for flight (-530 V). The data analysis was performed as follows:

- IDL (Interactive Data Language) [30d] scripts were written to fit the \(^{241}\text{Am}\) and \(^{57}\text{Co}\) spectra of each pixel for each temperature. As a consequence of the spectral fitting, the peak channels for the 59.5 keV and 122.1 keV peaks were obtained for each pixel, and the gain and offset values were obtained by a two point calibration using the relations below:

\[
(Ch_{122.1})_i = G_i \times (122.1) + O_i \quad (4.14)
\]

\[
(Ch_{59.5})_i = G_i \times (59.5) + O_i \quad (4.15)
\]

where \((Ch_{122.1})_i\) and \((Ch_{59.5})_i\) are the peak channels of 122.1 keV and 59.5 keV respectively, for the \(i\)th pixel; \(G_i\) and \(O_i\) is the gain and offset of the \(i\)th pixel.

The gain and offset are terms that define the linear relation between the channel number and energy (similar to the slope and intercept); gain and offset are in units of channel/keV and channel, respectively.

- Using the gain-offset values obtained for each pixel, the spectra for each pixel are converted from channel space to energy space. Due to the large amount of data, 100 pixels were randomly selected for each temperature. The energy spectra are fit with Gaussian functions (eqn(4.16)) to extract \(\sigma\) for each energy in units of keV.

\[
f(x) = A \times \exp \left[-\frac{(x - H)^2}{2\sigma^2}\right] \quad (4.16)
\]
where H is the peak energy, A is the maximum value (counts or count rate) at H and \( \sigma \) is the FWHM divided by 2.35, the ‘spectral width parameter’ in keV.

- The above steps are performed for all temperatures, and so the gain, offset and \( \sigma \)-energy relation for each pixel of the module are obtained as a function of temperature.

### 4.4.2.1 Variation of Channel number with temperature

The gain varies from pixel-to-pixel by 3%, while the offset varies by 10% for all temperatures. Since these variations lie within the 2\( \sigma \) confidence intervals, gain and offset values are averaged over all pixels, for each temperature, by computing the arithmetic mean. The variation of pixel averaged gain \( G_{pix}(T) \) and offset \( O_{pix}(T) \) with temperature is linear, and each data set is fit with a straight line. The best fit equations are given by

\[
G_{pix}(T) = 8.072 - (0.012)T \quad (4.17) \\
O_{pix}(T) = 491.08 + (0.051)T \quad (4.18)
\]

where T is the temperature in degrees C.

From these equations, it has been determined that there is a 1 channel increase, for every 1°C rise in temperature, after taking into account the entire energy range of operation.

### 4.4.2.2 Variation of Spectral Width Parameter with Energy and Temperature

Figure 4.9 shows three plots, each one representing one energy. The x-axis in each plot is the pixel number or ID and the y-axis is the \( \sigma \) in units of keV measured for that energy. The different symbols in each plot corresponds to a particular temperature (refer the legends). From the plots it is observed that

- there is minimal variation of \( \sigma \) among pixels
- for each energy, \( \sigma \) shows no observable temperature dependence
- pixel and temperature averaged \( \sigma \) shows no energy dependence

In order to understand these results, one must consider those factors that contribute to spectral line broadening in a detector. As discussed in chapter 1, the measured variance in the detected signal is given as the sum of the following components

\[
\sigma_{tot}^2 = \sigma_{Fano}^2 + \sigma_{ENC}^2 \quad (4.19)
\]
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Figure 4.9: Representation of the distribution of $\sigma$ (keV) with pixel number, for the three different energies. The different symbols represent $\sigma$ measured at different temperatures. The figures show minimal variation of $\sigma$ between pixels, and no visible energy or temperature dependence. **Top left:** $\sigma$ for 59.5 keV, the temperature averaged value is $2.36 \pm 0.41$ keV; **Top right:** $\sigma$ for 122.1 keV, the temperature averaged value is $2.35 \pm 0.57$ keV; **Bottom:** $\sigma$ for 136.5 keV, the temperature averaged value is $2.57 \pm 0.74$ keV.

where $\sigma^2_{\text{Fano}}$ is the contribution to spectral line broadening due to statistical fluctuations in the number of charge carriers produced by incident radiation, and $\sigma^2_{\text{ENC}}$ is the contribution due to electronic noise, or ENC (refer section 1.1.3) in units of number of electrons. These terms are expressed mathematically in units of (keV)$^2$ by

$$\sigma^2_{\text{Fano}} = FEW$$  \hspace{1cm} (4.20)

$$\sigma^2_{\text{ENC}} = W^2(\text{ENC})^2$$  \hspace{1cm} (4.21)
As discussed earlier, the spectral width parameter, $\sigma(E)$, is the square root of $\sigma^2(E)_{tot}$, and can be written in terms of its constituents as

$$\sigma = \sqrt{\sigma^2_{tot}} = \sqrt{\sigma^2_{Fano} + \sigma^2_{ENC}} = \sqrt{(FW) + W^2(ENC)^2}$$  \hspace{1cm} (4.22)

where $F$ is the Fano factor of the material, $E$ is the energy of the photon, $W$ is the minimum energy required to create an electron-hole pair in the detector. $F$ is experimentally measured for the AMPTEK CdTe detector (section 2.4.1) and this value is used for the CZT detector in this calculation; the value of $W$ is taken as that given by the manufacturers (see table(4.2)). These two parameters are frozen for the fit. For each temperature, data corresponding to pixel averaged $\sigma$ versus energy were fitted using eqn(4.22), and the value of ENC was extracted as the best fit parameter. The ENC values extracted from the fit for each temperature using the equation show no dependence on temperature. Leakage current for these detectors show a slow exponential decrease with decrease in temperature, but this has been washed out by some temperature independent component. The source of this noise could be the ASICs that are bonded to the CZT detector. After averaging over temperature the ENC value is, 510 electrons.

In order to illustrate the effects of the ENC on the energy dependence of $\sigma$, consider fig(4.10). It shows the contribution of ENC and inherent statistical fluctuations to the measured spectral width, as a function of energy. The measured values (black points) are pixel-averaged values for 0°C, and the error bar on each point is the standard deviation. If the dominant source of peak broadening was due to statistics of charge generation in the CZT detector (calculated using eqn(4.21)), then the $\sigma$ values would show an energy dependence $\sigma_{Fano}$, as shown by the blue points in the graph. The horizontal line represents the $\sigma_{ENC}$ due to the ENC alone (calculated using eqn(4.21), using the experimentally measured value of 510 electrons); the measured $\sigma$ values are the quadrature sum of $\sigma_{Fano}$ and $\sigma_{ENC}$. As seen, the ENC dominates the measured $\sigma$ values, washing out the energy dependence. This is the case for all temperatures.

To summarize

- Channel number increases by one unit ($\sim$70 eV for this system) for every $1^\circ$ rise in temperature.
- $\sigma$ shows no energy dependence or significant variation with temperature. Pixel-to-pixel variation of this parameter is minimal and can be neglected for all practical purposes.
The energy dependence and temperature dependence of $\sigma$ is smeared out by a dominant, temperature independent source of electronic noise. This is attributed to a non-thermal noise component arising from the ASICs.

The data obtained from laboratory characterization of the detector was used to extract the $(\mu \tau)_{e,h}$ which are important for modeling the detector SRF. Spectra obtained during detector calibration were used to measure spectral parameters like gain, offset and $\sigma$ and study their behavior with energy and temperature. The final response matrix will however have to be constructed using data measured by the CZT in the flight configuration.

The HEX payload was characterized in a thermovacuum chamber with purpose of monitoring its operation in vacuum with varying temperatures. As part of the procedure, the CZT detectors were calibrated and the events were processed and stored using the flight electronics.

The next section discusses the results obtained after analysis of data measured during calibration in the thermovacuum chamber.
4.5 Results from the Thermovacuum calibration of module B11290

HEX was placed in a thermovacuum chamber and cycled through a temperature range of -20°C to +45°C for a period of 10 days under a vacuum of a few $10^{-5}$ torr in order to assess the performance of the payload under a simulated space environment. The CZT detectors were powered on only between temperature limits of -20°C to +15°C. This thermal range of operation was constrained due to CZT array temperature limits. Unlike the laboratory calibration which was done individually for the bare crystals using the electronics provided by IDEAS (section 1.2.2), during the thermovacuum calibration

- all nine detector modules were mounted on the same board and were simultaneously biased from a common power supply developed as part of the payload
- all associated locally developed electronics were also mounted in the actual flight configuration
- the power was supplied via DC/DC converters as expected during actual operation in space
- the stainless steel collimator was mounted in front of the CZT detector array; the radiation used to calibrate the detectors was thus modulated by the collimator response before incidence on the detectors.

The data measured by the module B11290 was reduced and analyzed as described in section 4.4.2.

The channel-energy relation expressed by eqn(4.23) was used to extract the gain and offset for different temperatures.

Channel = \( \frac{\text{Energy}}{\text{Gain} \times 10^{-3}} + \text{Offset} \) \hspace{1cm} (4.23)

where gain and offset are in units of eV/channel and channel, respectively.

Gain and offset were extracted for each pixel for every temperature. The pixel-to-pixel variations of the gain and offset were not very significant and so were averaged over all pixels. Thus, for every temperature, there is a pixel-averaged value of gain and offset, \( G_{\text{pix}} \) and \( O_{\text{pix}} \) and the equations (4.24) and (4.25) express the temperature dependence of these two parameters

\[
G_{\text{pix}}(T) = 192.7 + (0.256)T \quad \text{eV/channel} \hspace{1cm} (4.24)
\]

\[
O_{\text{pix}}(T) = -85.47 + (1.76)T \quad \text{channel} \hspace{1cm} (4.25)
\]
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where $T$ is the temperature measured in degrees C.

These equations show that the channel number increases by one unit (~244 eV for this system) for every degree rise in temperature, which is consistent with what was seen from the laboratory calibration.

**Figure 4.11:** These plots are $\sigma$-histograms; the $\sigma$ (keV) values for pixels are binned. **Top:** $\sigma$-histograms for 30.97 keV, 81 keV, and 122.1 keV, measured at a temperature of 11°C; the average $\sigma$ values show no dependence on energy; **Bottom:** $\sigma$-histograms for 59.5 keV and 122.1 keV measured at a temperature of -5°C; there is still no energy dependence seen. Also note that there is no difference between the mean $\sigma$ of 122.1 keV measured at high and low temperatures.

Figure 4.11 shows two plots which are $\sigma$-histograms; these are constructed by binning $\sigma$ (keV) values of all pixels, for each energy. The $\sigma$-histograms are plotted here for 30.97 keV.
keV, 81 keV, and 122.1 keV at a temperature of $11^\circ$C. As can be seen, the graphs follow a Gaussian distribution, and it is evident that for each energy, the peaks of the Gaussian lie at the same value on the x-axis. This indicates that the mean $\sigma$ value for each of the energies is the same, within errors. $\sigma$-histograms are also plotted for 59.5 keV and 122.1 keV at $-5^\circ$C; once again it can be seen that the peaks of the distributions lie at the same value. Also, the mean value of $\sigma$ computed for 122.1 keV shows no difference between higher and lower temperatures. From this one can observe that the energy and temperature dependence of $\sigma$ have been smeared out by a dominant noise factor.

Equation (4.22) was used to fit pixel and temperature averaged $\sigma$ values versus energy to extract the ENC value in units of number of electrons, and this value was found to be $818 \pm 27$ electrons. As was depicted in fig(4.10), the dominant effect of ENC on the measured value of $\sigma$ during thermovacuum calibration is shown in fig(4.12). From the above study, it is clear that the contribution of this temperature independent noise is larger when measurements are made with the flight electronics. The average $\sigma$ measured using thermovacuum data is larger by a factor of 1.5 compared with the average $\sigma$ measured using laboratory data. Potential sources of this noise include the power line noise from the DC-DC converters.

The next section discusses simulation of the CZT detector response using the spectral parameters extracted from experimental data.

Figure 4.12: This plot shows the effect of ENC on the value of $\sigma$. The x-axis is the energy (keV). The black points are the experimentally measured values of $\sigma$, and the open squares are what the measurements would have been if the only contribution were from statistical fluctuations of charge generation. The ENC contribution is shown by the solid red line, which corresponds to $818 \pm 27$ electrons.
4.6 Simulation of CZT detector response

The previous sections described the analysis of data from laboratory and thermovacuum calibrations of CZT module B11290, and discussed the important conclusions that could be drawn from the results. The main aim of this exercise is to simulate the SRF of the CZT detector over the entire energy range. The first step towards this is to simulate source spectra corresponding to laboratory calibration and validate the modeled spectra against experimental measurements of the same. This is a requirement in order to establish confidence in the procedure adopted.

A Geant4 application was designed to simulate the SRF for the pixels of a single CZT module as per laboratory calibration. The simulation was to be run for different temperatures for high energy photons of the radioactive source $^{57}$Co.

A simple model of the detector geometry was chosen. The CZT detector was made sensitive by setting the pointer of the object of the CZT sensitive detector class to its logical volume. The energy deposited in the CZT detector was obtained by extracting the hits information in the UserEventAction class via the object of the G4HCofThisEvent class.

The source geometry was simulated using the GSPM. During laboratory calibration, the source was positioned such that all pixels were uniformly illuminated. For the simulation, this source arrangement was approximated; a square plane source was used with a parallel photon beam in order to simulate uniform illumination. The physical processes included are listed in table 2.3.

Since the energy deposit in the CZT is extracted in the UserEventAction class, one must include the following as input to this class in order to modulate the absolute energy deposit:

- the pixel, energy and temperature averaged $\sigma$ which will be used to induce spread to the absolute energy deposit
- temperature dependent energy-channel conversion equation
- individual $(\mu\tau)_e$ and $(\mu\tau)_h$ values for every pixel, for each temperature

The radioactive source $^{57}$Co was simulated in GSPM. The application was executed for the six different temperatures, with each execution consisting of $10^6$ events.

The flow of logic that is used for the response simulation, implemented in the UserEventAction class is as follows:
consider the first simulation run for temperature T\textdegree{}C and pixel p_1; the (μτ)_{e,h} for this temperature and pixel are entered as input to the application

when a photon of energy E interacts with the detector, its total energy deposit and depth of interaction are extracted using the object of hits collection in the UserEventAction class; this is the first event

the Hecht equation (eqn(4.13)) is part of the code, and the depth of interaction for this event is input into the equation and the CCE η for the event is obtained as a result

σ is hard coded into the application as a constant value which has no energy or temperature dependence

E and σ are passed as arguments to the function G4RandGauss, which generates a Gaussian energy distribution using E as the mean value and σ as the spread

this function then randomly selects a value of energy from the distribution, and this is returned as the output of the function

this value is now the energy deposited in the detector which includes the inherent statistical fluctuations and electronics noise which was contained within σ; let this energy be represented by E_{smear}

E_{smear} is then multiplied by the η for the event; then the final energy deposit, E_{final} is obtained, which now includes the effects of charge collection

for temperature T\textdegree{}C, the gain and offset are computed using equations (4.24) and (4.25); then the gain, offset and E_{final} are input into eqn(4.23), where the channel number Ch_{final} for that event is obtained

in this way, Ch_{final} corresponding to each event is generated and these channel numbers are written into a file

at the end of the run, the file containing the channel number is binned to generate a pulse height spectrum, which is the SRF

this procedure is repeated for different temperatures; the simulated results are validated against experimentally measured SRF

The simulated and experimental spectra are normalized and represented in units of probability per unit channel. The parameters used for validating the simulated and experimental results are

- Overall spectral shape
• Reproducibility of the peak channel numbers
• Reproducibility of the spectral width parameter ($\sigma$)

The results of the simulation are shown in fig(4.13) for four randomly selected pixels, each at a particular temperature.

As can be seen from these plots, there is good agreement between experimental data and the simulated pulse height spectra. According to the legends in the figures, one can see that irrespective of the location of the pixel within the detector module, or the temperature at which the measurements were made,

1. the experimentally extracted values of $(\mu \tau)_{e,h}$ products are correct within uncertainties as the peak normalization and the exponential low energy tail are very well matched for the selected pixels and for the temperatures.

2. the good match between experimental and simulated data support the assumptions made regarding the pixel-to-pixel variation and temperature dependence of spectral parameters

From the simulation of the CZT detector response using spectral parameters extracted from laboratory data, there is ample confidence in the methodology to take the work to the next level, which is the simulation of the detector response using the spectral parameters extracted from thermovacuum calibration data and the generation of the SRF for all energies within the 30-270 keV range.

As discussed earlier, the CZT detector response simulation relies on a procedure set up for generation of the SRF for the detector within the 30-270 keV region. Figure(4.14) shows the simulated SRF for the entire CZT detector, taking into account the $(\mu \tau)_{e,h}$ averaged for each pixel, and the spectral parameters extracted using the data measured with the flight electronics at 11°C in the thermovacuum chamber. The SRF has been generated for three $\gamma$-ray lines, 30.97 keV, 81 keV, and 122.1 keV. Similarly, the SRF can be generated for any $\gamma$-ray line within the energy range of interest. The y-axis corresponds to the probability that an incoming photon energy $E$ is redistributed into channel ‘i’. These values, when generated for all the energies, can then be used to populate a two-dimensional matrix with the rows representing energies and columns representing channel number. The SRF is represented in a tabular form or in the form of a two-dimensional matrix as shown in table(4.3), where $E_j$ represents the energy from 30-270 keV (j), Ch represents the channel number from 0 to 1023 (i), and $p_{j,i}$ is the probability that $E_j$ is measured in Ch$_i$. Connecting table(4.3) to fig(4.14), one can see that 30.97 keV is $E_1$ and the numbers from $p_{1,1}$ to $p_{n,1}$ are the probability values for
Figure 4.13: Reproduction of experimentally measured CZT detector response with Geant4 using spectral parameters extracted from analysis of experimental data. Solid lines represents simulated values, while black points represent experimentally measured values.
Table 4.3: Tabular representation of the Spectral Redistribution Function (SRF)

<table>
<thead>
<tr>
<th>Channel→ Energy(keV)↓</th>
<th>Ch$_1$</th>
<th>Ch$_2$</th>
<th>Ch$_3$</th>
<th>\ldots</th>
<th>Ch$_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$</td>
<td>$p_{1,1}$</td>
<td>$p_{1,2}$</td>
<td>$p_{1,3}$</td>
<td>\ldots</td>
<td>$p_{1,n}$</td>
</tr>
<tr>
<td>$E_2$</td>
<td>$p_{2,1}$</td>
<td>$p_{2,2}$</td>
<td>$p_{2,3}$</td>
<td>\ldots</td>
<td>$p_{2,n}$</td>
</tr>
<tr>
<td>$E_3$</td>
<td>$p_{3,1}$</td>
<td>$p_{3,2}$</td>
<td>$p_{3,3}$</td>
<td>\ldots</td>
<td>$p_{3,n}$</td>
</tr>
<tr>
<td>\vdots</td>
<td>\vdots</td>
<td>\vdots</td>
<td>\vdots</td>
<td>\vdots</td>
<td>\vdots</td>
</tr>
<tr>
<td>$E_n$</td>
<td>$p_{n,1}$</td>
<td>$p_{n,2}$</td>
<td>$p_{n,3}$</td>
<td>\ldots</td>
<td>$p_{n,n}$</td>
</tr>
</tbody>
</table>

30.97 keV from channel 0 to 1023. Similarly, 81 keV is $E_2$, and 122.1 keV is $E_3$. At the present time, the generation of the SRF represented in Fig(4.14) was done using pixel averaged values of $(\mu \tau)_{e,h}$. At a later stage one would like to incorporate the individual pixel $(\mu \tau)_{e,h}$ values and determine the difference between the two by comparison with actual experimental data. This comparison would help in determining whether the approximation of pixel averaged $(\mu \tau)_{e,h}$ products produces any significant variations.
4.7 Summary and Conclusions

1. The aim of this chapter is to simulate the response of the CZT detector so as to generate the detector spectral redistribution function (SRF). This is the first step to construction of the response matrix, and was demonstrated.

2. The signal generation in CZT detectors and the effect of charge trapping on the signal pulse height was studied.

3. Using CZT spectral data measured in the laboratory at different operating voltage, $(\mu\tau)_{e,h}$ were extracted for different temperatures using a spectral fitting routine written in IDL. These parameters were extracted for different temperatures for all the pixels of the CZT detector module under study.

4. The variation of the mobility-lifetime products with temperature was studied by taking into consideration the pixel-averaged values. For every $5^\circ$C variation in temperature, the $(\mu\tau)_e$ values vary by 0.7% while the $(\mu\tau)_h$ values by 2.3%.

5. Independent data analyses were performed on the CZT detector spectra measured in the laboratory with vendor supplied ground electronics and in the thermovacuum chamber with custom built flight electronics and the differences in the spectral parameters extracted were studied. The most important observation was the measured value of $\sigma$

   - In both sets of data it was observed that there was no energy dependence or temperature dependence of $\sigma$.
   - **Laboratory Data** - Average $\sigma = 2.4$ keV, ENC = 510 electrons
   - **Thermovacuum Data** - Average $\sigma = 3.8$ keV, ENC = 819 electrons

   It may be concluded that the energy dependence of $\sigma$ was washed out by a dominant noise term that showed no dependence on temperature. As can be seen, measurements made with the flight electronics in the thermovacuum chamber shows a higher incidence of noise.

6. Using these inputs from experimental data, the CZT detector response was successfully simulated. The confidence gained in reproducing experimental data for individual pixels and for different temperatures lead to the simulation of the detector SRF.
Bibliography


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