

Statistical Modeling of Carrier Transport and Scattering in Cryogenic Dark Matter Detectors

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Abstract

The Super Cryogenic Dark Matter Search (SuperCDMS) experiment uses cryogenic, solid-state detectors to infer the nature of particle interactions in a rare-event search for particles which may constitute dark matter. The experiment relies on the Geant4 Condensed Matter Physics (G4CMP) package to model and understand the underlying physics that compels the response of the solid-state detectors. The G4CMP simulation models solid-state excitations and their relevant processes which includes the transport and scattering of charge carriers and phonons. This report validates that G4CMP's Monte Carlo method for modeling charge carrier and phonon physics is in agreement with the theoretical description as well as evaluates the CPU cost of different processes. We conclude that further investigation is required to confirm the source of CPU consumption with the addendum that the simulation may be further optimized by migrating from a single-scatter model to a multiple-scatter model.

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Chapter 1

Introduction

1.1 Overview of this Report

In this report, we aim to investigate the modeling of charge carrier and phonon physics in the SuperCDMS experiment's G4CMP-based detector response simulation as well as explore opportunities for optimization. We start in Chapter 1 with an introduction to the SuperCDMS experiment, relevant detector physics, and the purpose and description of the G4CMP-based simulation. In Chapter 2, we provide an overview of the theoretical description of carrier and phonon physics in solid-state devices to establish a baseline of expected behavior from the simulation. In Chapter 3, we start by providing an overview of the Monte Carlo method and tracking in Geant4 which sets us up to compare the simulation's model of carrier and phonon physics to the expectations established in Chapter 2. We then investigate CPU time consumption as a function of carrier and phonon processes. We end with a discussion of future work which may involve the use of statistical modeling in place of single-scatter modeling as a way to optimize CPU time.

1.2 The SuperCDMS Experiment at SNOLAB

The Super Cryogenic Dark Matter Search (SuperCDMS) experiment is a next-generation experiment that aims to directly detect low-mass particles ($\leq 10 \text{ GeV}/c^2$) which may constitute dark matter. The experimental setup includes cryogenic, solid-state detectors composed of two target materials: germanium and silicon. The experiment is located nearly 2 km underground within SNOLAB in Ontario, Canada which boasts a 6010 meter water equivalent overburden, shielding from cosmic-ray secondaries [1].

The detectors are instrumented on each side with phonon sensors ar-

ranged in channels. In addition, they may also be instrumented with charge readout sensors that, when coupled with the phonon measurement, enables the ability to distinguish between electron and nuclear recoils through a measurement of the ratio between ionization energy and the total recoil energy (ionization yield) [1, 2]. The detectors may also utilize a voltage bias up to ~ 100 V to amplify the phonon signal (discussed in further detail in the next section) and lower the energy threshold for detection of recoils to probe particles in the mass range $\lesssim 4$ GeV/c² but are unable to distinguish between recoil type [1, 3].

1.3 Detector Physics

The SuperCDMS detectors infer particle interactions through the production and collection of charge carriers and phonons. Provided the detectors are operated at cryogenic temperatures, no ionization occurs through thermal excitations which ensures the region is depleted of free charge carriers.

1.3.1 Charge and Phonon Production

A typical energy deposit, as shown in Fig. 1.1, results in the liberation of charge carriers which are transported to either surface under a bias voltage provided by the electrodes [4].

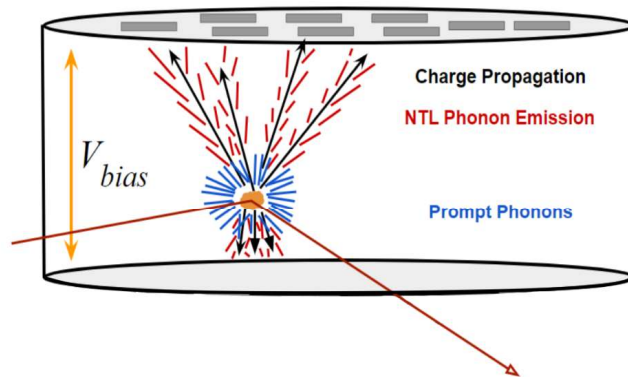


Figure 1.1: Diagram of an energy deposit resulting in the recoil of electrons or nuclei. Liberated electrons and holes initially emit prompt (primary) phonons before they travel under voltage to opposite surfaces. The work done by the field is radiated in the form of Luke phonons (NTL emission). Image courtesy of SuperCDMS Collaboration.

The expected number of charge pairs produced is given by the expres-

sion

$$n_{eh} = Y \frac{E_{recoil}}{\epsilon_{eh}}, \quad (1.1)$$

where E_{recoil} is the recoil energy of the nucleus, Y is the ionization yield, and ϵ_{eh} is the average electron-hole pair energy [5]. The expected phonon energy produced is then given by

$$E_{Ph} = E_{recoil} + n_{eh} \cdot e \cdot \Delta V \quad (1.2)$$

$$= E_{primary} + E_{Luke}, \quad (1.3)$$

where e is the fundamental charge of the electron and ΔV is the bias voltage of the detector. The first term $E_{primary} = E_{recoil}$ represents the primary phonon energy [1]. It is the phonon energy emitted by the electrons and holes shortly after their liberation [4]. Once the electrons and holes have lost enough energy, the force provided by the electric field can do work by transporting them to the surface. There is a phonon energy gain from the field which arises from the Neganov-Trofimov-Luke (NTL) effect and is expressed as $E_{Luke} = n_{eh} \cdot e \cdot \Delta V$ [1, 6, 7].

1.3.2 Charge Readout

As the liberated charge carriers move under voltage, their motion induces an instantaneous current i on the charge sensor electrode given by

$$i = E_v e v, \quad (1.4)$$

where e is the fundamental electron charge, v is the electron's velocity, and E_v is the electric field produced by the electrode in the direction of velocity v under the conditions: electron removed, given electrode raised to unit potential, all other electrodes grounded [8, 9].

The induced current arises from the time derivative of an image charge on the plate of the capacitor seen in the left figure in Fig. 1.2 (labeled as “sensor”) [12]. The induced charge on the electrode q_{in} is negated with a feedback charge q_f injected by the amplifier through its feedback network. The output voltage V_{out} seen in the right figure of Fig. 1.2 is driven by the feedback charge sent through the feedback capacitor C_f [4].

1.3.3 Phonon Collection

The produced phonons may propagate until they are collected by the phonon sensors, quasiparticle-trap-assisted electrothermal-feedback transition edge sensors (QETs), instrumented on the surface. The majority

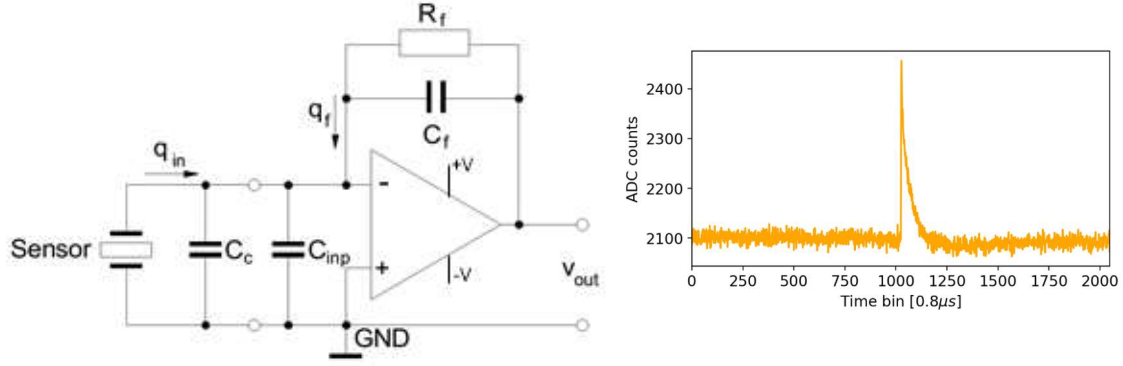


Figure 1.2: **Left:** Simplified diagram of a charge amplifier where the detector serves as the capacitor labeled as “sensor”. Figure reproduced from Ref. [10]. **Right:** Typical charge circuit response to the change in detector capacitance for a real event. Figure adapted from Fig. 3.5 in Ref. [11].

of phonons are absorbed into the aluminum fin of the QET shown in the left figure of Fig. 1.3. The aluminum energy gap ($\sim 350 \mu\text{eV}$) serves to separate the athermal phonon signal from the ambient thermal phonon population, as a phonon’s energy must be above $2\times$ the energy gap to be absorbed and break a Cooper pair and liberate quasiparticles [13]. The liberated quasiparticles may then enter the aluminum/tungsten overlap region where they experience a suppressed energy gap which allows them to convert their potential energy into kinetic energy or into the potential energy of a higher number of tungsten excitations [14].

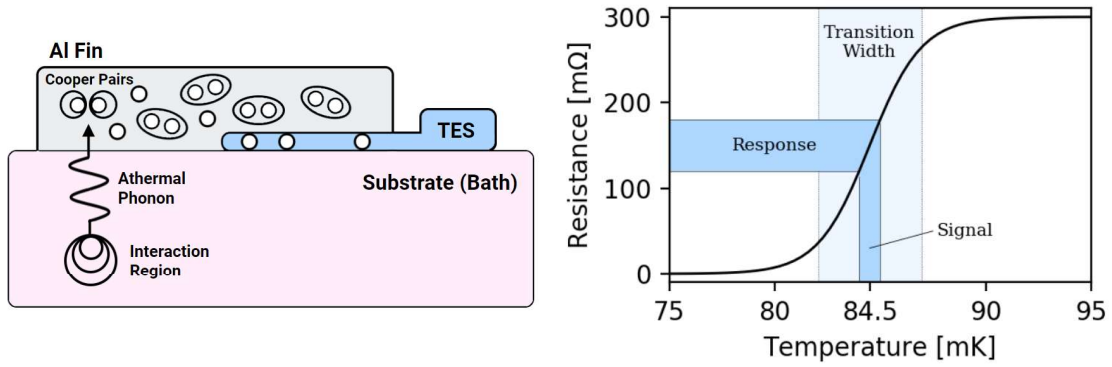


Figure 1.3: **Left:** Cross-section of the interface between the detector substrate (pink), the aluminum fin (grey) and the tungsten TES (blue). **Right:** An example superconducting transition region of a TES in which the resistance of the tungsten rapidly rises with temperature before going normal.

1.3.4 Phonon Readout

The tungsten TES is held at its superconducting transition temperature, shown in the right figure of Fig. 1.3, during its operation which yields a steep relationship between its resistance and its temperature. The TES's resistance increase due to a small increase in temperature is utilized by the circuit to the left in Fig. 1.4 to detect small temperature changes from phonon absorption. The circuit is designed such that the TES is voltage biased which ensures stable operation in a negative electro-thermal feedback loop [15]. The change in current through the TES resulting from phonon absorption is sensed with cryogenic amplifiers (not pictured) which produce the signal seen to the right in Fig. 1.4 [13].

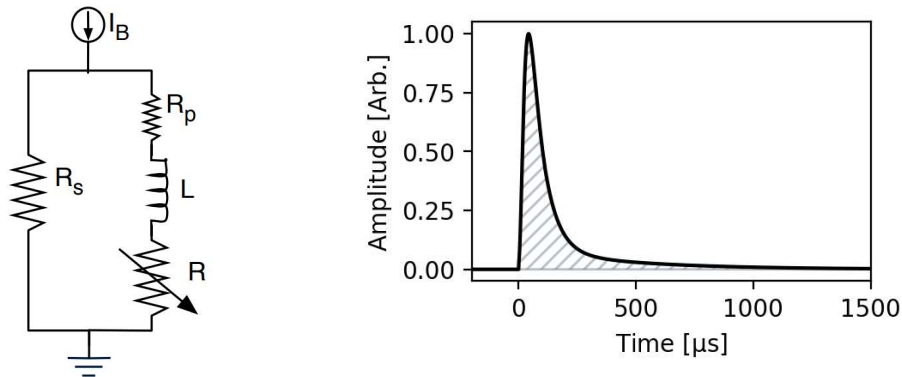


Figure 1.4: **Left:** Simplified diagram of the TES circuit containing a current source I_B , a shunt resistor R_s , parasitic resistance R_p , an inductor L , and the TES R labeled as a variable resistance. Figure adapted from Fig. 3.5 in Ref. [14]. **Right:** Phonon signal template of change in current amplitude as a function of time constructed from experimental data. Template was first published in Fig. 9 in Ref. [16].

In the next section, we discuss how the physics processes mentioned in this section are implemented in a detector response simulation.

1.4 G4CMP-Based Detector Response Simulation

The Geant4 [17–19] Condensed Matter Physics (G4CMP) package is a tool for simulating the passage of particles through matter at cryogenic temperatures using solid-state non-equilibrium excitations. The package introduces charge carriers and phonons as well as their associated processes whose stochastic behavior is modeled with a Monte Carlo transport method [16].

In addition to the simulation of charge and phonon production, transportation, and scattering in a SuperCDMS detector, G4CMP includes a

lumped, “zero-dimensional” simplification of Kaplan’s model of phonon-electron interactions in superconductors to model the collection of phonon energy incident on the QET [16, 20]. The phonon arrival power spectrum is then used as an input parameter to a SuperCDMS-specific circuit model (TESSim) which translates the collected phonons into a signal similar to the right figure of Fig. 1.4 [21]. In later stages, realistic noise is added and the signals are converted to the same format as the experiment’s “raw” data. Finally, the simulated signals are processed through the reconstruction software the same way as experimental data [22].

A direct comparison between the reconstructed quantities of both then reveals how well our understanding of the detector physics compares to the true detector response. A comparison also allows us to infer what processes contribute to the final data points as well as what physical assumptions are appropriate for analysis [22].

In the next chapter, we take a closer look at a theoretical description of charge carrier and phonon physics in a solid-state device before comparing to the Monte Carlo approach used in G4CMP.

Chapter 2

Theoretical Description of Carrier and Phonon Physics

2.1 Potentials in Semiconductor Medium

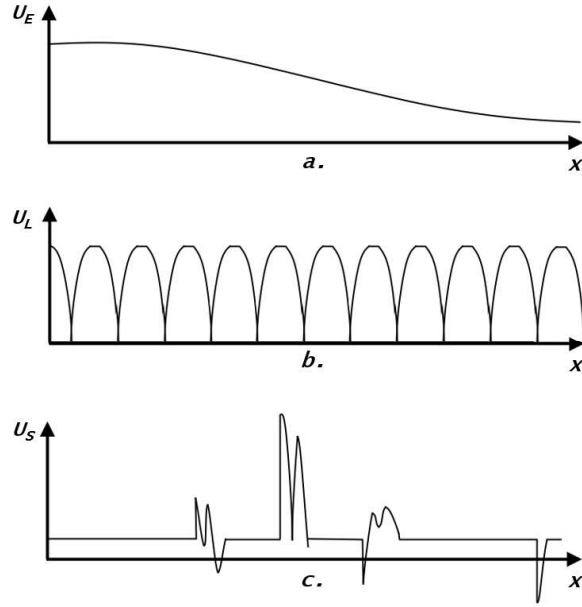


Figure 2.1: Illustration of the three types of potentials which contribute to the Schrödinger equation in a crystal. **a.** shows an externally applied potential field U_E which may not be uniform in space. **b.** shows a periodic potential field U_L from the crystal lattice. **c.** shows a random potential U_S which arises from lattice deformation or impurities. Figure adapted from Fig. 2.1 in Ref. [4].

A description of an electron in a potential $U(\mathbf{r}, t)$ is given by the one-electron Schrödinger equation

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m_0} \nabla^2 \Psi(\mathbf{r}, t) + U(\mathbf{r}, t) \Psi(\mathbf{r}, t), \quad (2.1)$$

where m_0 is the mass of the free electron and the electron wave-function $\Psi(\mathbf{r}, t)$ is a solution to the equation. Let's define $U(\mathbf{r}, t)$ such that it is the sum of the three potentials illustrated in Fig. 2.1.

$$U(\mathbf{r}, t) = U_E(\mathbf{r}) + U_L(\mathbf{r}) + U_S(\mathbf{r}, t), \quad (2.2)$$

where $U_E(\mathbf{r})$ is a potential which describes an externally applied electric field. $U_L(\mathbf{r})$ describes a periodic potential of a perfectly static crystal lattice. $U_S(\mathbf{r}, t)$ describes the scattering or deformation potential which arises from impurities or random fluctuations of the lattice nuclei [23].

2.1.1 External Potential

By neglecting the lattice potential and scattering potential from Eq. 2.1, we arrive at a solution for a simple one-dimensional case through the separation of variables

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m_0} \nabla^2 \Psi(x, t) + U_E(x) \Psi(x, t) \quad (2.3)$$

$$\Psi(x, t) = a_k e^{\pm i k x} e^{-i \omega t}; \quad k^2 = 2m_0(E - U_E)/\hbar^2; \quad \omega = E/\hbar \quad (2.4)$$

where E , the separation variable, is representative of the particle's energy and a_k is an arbitrary constant [24, 25]. The solution to this equation $\Psi(x, t)$ describes a wave packet with its wave-vector centered on k and its frequency centered on ω . Classical wave theory then yields the relationship for the group velocity of the wave packet [26]

$$v_g = \frac{d\omega}{dk} = \frac{1}{\hbar} \frac{dE}{dk} \quad (2.5)$$

The momentum of the wave packet provided by its group velocity $m_0 v_g$ is different but related to the quasi- or crystal momentum $\hbar k$ by the following [26, 27]

$$m_0 v_g = \hbar k \quad (2.6)$$

We now move to finding an expression for the electron's effective mass m^* under the force of an electric field. The force that the charge experiences in a field can be described by using the time derivative of the quasi-momentum [4, 26]

$$\mathbf{F} = -\nabla U_E = \frac{d(\hbar \mathbf{k})}{dt} \quad (2.7)$$

The magnitude of the force is related to the time derivative of the group velocity of the wave packet

$$|\mathbf{F}| = m^* \frac{dv_g}{dt} \quad (2.8)$$

Using the expression in Eq. 2.5, the time derivative of the group velocity can be written in a suggestive form

$$\frac{dv_g}{dt} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2} \frac{\partial(\hbar k)}{\partial t} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2} |\mathbf{F}| \quad (2.9)$$

which reveals an expression for the effective mass of an electron

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2} \quad (2.10)$$

This result is significant, as it indicates that an electron will appear to have a mass that depends on the dispersion relationship in Eq. 2.5 which is material-dependent [26]. In the next section, we explore the behavior of electrons and holes in the periodic potential of a crystal lattice.

2.1.2 Periodic Lattice Potential

We now neglect all potentials except the periodic potential and write our new equation as

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m^*} \nabla^2 \Psi(\mathbf{r}, t) + U_L(\mathbf{r}) \Psi(\mathbf{r}, t) \quad (2.11)$$

We have replaced the mass of a free electron m_0 with the effective mass m^* to accommodate the case in which the E - k relationship is not constant as seen by the energy band structure in the right figures of Fig. 2.2 [26].

We take the simple case that the potential is periodic with a lattice that has equal spacing a in one dimension

$$U_L(x) = U_L(x + na); n \in \mathbb{Z} \quad (2.12)$$

Bloch's theorem is then applied to arrive to the general solution

$$\Psi(x, t) = u_{n,\mathbf{k}} e^{\pm i k x} \quad (2.13)$$

, where the function $u_{n,\mathbf{k}}$ is periodic with the lattice spacing

$$u_{n,\mathbf{k}}(x) = u_{n,\mathbf{k}}(x + na); n \in \mathbb{Z} \quad (2.14)$$

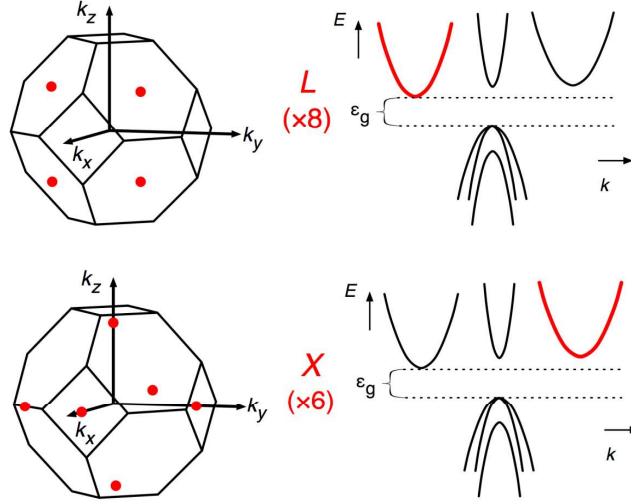


Figure 2.2: **Top:** The germanium L -valley directions in k -space (**Left**) and the L -valley highlighted in the energy band structure for germanium (**Right**). **Bottom:** The silicon X -valley directions in k -space (**Left**) and the X -valley highlighted in the energy band structure for silicon (**Right**). Figures adapted from Fig. 2.2 in Ref. [4].

It should be noted that the function $u_{n,\mathbf{k}}$ is different for each band n and wave-vector $\mathbf{k}$ [25, 28].

An interesting consequence that arises from the anisotropy in the relationship of E to k in k -space is that under a small electric field, electrons may move oblique to the direction of the field's force [21]. The conduction band energy minima of a crystal are known as valleys. The valleys in germanium and silicon have ellipsoid equal energy surfaces such that the energy in the valley frame can be written as

$$E = \frac{\hbar^2}{2} \left(\frac{k_x^2}{m_l} + \frac{k_y^2}{m_t} + \frac{k_z^2}{m_t} \right) \quad (2.15)$$

which implies that electrons under forces in the longitudinal (transverse) direction of the valley respond as if they had a longitudinal (transverse) mass m_l (m_t) [29]. The longitudinal and transverse masses are shown in Table 2.1.

	Ge	Si
m_l/m_e	1.588	0.91
m_t/m_e	0.081	0.19

Table 2.1: Effective electron masses in germanium and silicon in units of the free electron mass m_e . Values taken from G4CMP crystal configuration files [30].

At the start of each charge track, the charge is assigned to a valley [16]. We can then find our equation of motion $\mathbf{a} = \mathbf{m}^{*-1}\mathbf{F}$ in the valley frame where the inverse mass tensor $\mathbf{m}^{*-1}$ is diagonalized [4]. The following derivations, using the guidance of Iman Atae Langroudy's work [31], exemplify charge kinematics in germanium and silicon valleys.

As shown in Fig. 2.2, a germanium valley we can work with is in one of the L directions $\mathbf{k}_L = \frac{1}{\sqrt{3}}(1, 1, 1)$. We also define the direction of the force of the electric field with $\mathbf{F} = (0, 0, F)$. To simplify our calculations, since we are only concerned with oblique transport with respect to the field direction, let's consider a frame such that the valley direction is in the xz -plane: $\mathbf{k}_L = \frac{1}{\sqrt{2}}(1, 0, 1)$. Let's now make the coordinate transformation on the force vector such that the x -axis is pointing in the same direction as the valley:

$$\mathbf{F}^* = \begin{bmatrix} \cos(\pi/4) & 0 & \sin(\pi/4) \\ 0 & 1 & 0 \\ -\sin(\pi/4) & 0 & \cos(\pi/4) \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ F \end{bmatrix} = \begin{bmatrix} F \sin(\pi/4) \\ 0 \\ F \cos(\pi/4) \end{bmatrix}$$

We can now calculate the acceleration in the valley frame

$$\mathbf{a}^* = \begin{bmatrix} \frac{1}{m_l} & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_t} \end{bmatrix} \begin{bmatrix} F \sin(\pi/4) \\ 0 \\ F \cos(\pi/4) \end{bmatrix} = \begin{bmatrix} \frac{F}{m_l} \sin(\pi/4) \\ 0 \\ \frac{F}{m_t} \cos(\pi/4) \end{bmatrix}$$

and transform back into the global frame

$$\mathbf{a} = \begin{bmatrix} \cos(-\pi/4) & 0 & \sin(-\pi/4) \\ 0 & 1 & 0 \\ -\sin(-\pi/4) & 0 & \cos(-\pi/4) \end{bmatrix} \begin{bmatrix} \frac{F}{m_l} \sin(\pi/4) \\ 0 \\ \frac{F}{m_t} \cos(\pi/4) \end{bmatrix} = \begin{bmatrix} \frac{F}{2m_l} - \frac{F}{2m_t} \\ 0 \\ \frac{F}{2m_l} + \frac{F}{2m_t} \end{bmatrix}$$

Using our values for m_l and m_t from Table 2.1, we find the acceleration is in the direction $\mathbf{a} = (-5.86, 0, 6.49)F/m_e$. Despite what the name suggests, electrons do not necessarily travel along the valley direction.

Let's choose a silicon valley $\mathbf{k}_X = (0, 0, 1)$ aligned with the field $\mathbf{F} = (0, 0, F)$. We transform the force vector according to the coordinate system rotation that aligns the valley with the x -axis:

$$\mathbf{F}^* = \begin{bmatrix} \cos(\pi/2) & 0 & \sin(\pi/2) \\ 0 & 1 & 0 \\ -\sin(\pi/2) & 0 & \cos(\pi/2) \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ F \end{bmatrix} = \begin{bmatrix} F \\ 0 \\ 0 \end{bmatrix}$$

which results in an acceleration of

$$\mathbf{a}^* = \begin{bmatrix} \frac{1}{m_l} & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_t} \end{bmatrix} \begin{bmatrix} F \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{F}{m_l} \\ 0 \\ 0 \end{bmatrix}$$

We then transform back into the global frame to find

$$\mathbf{a} = \begin{bmatrix} \cos(-\pi/2) & 0 & \sin(-\pi/2) \\ 0 & 1 & 0 \\ -\sin(-\pi/2) & 0 & \cos(-\pi/2) \end{bmatrix} \begin{bmatrix} \frac{F}{m_l} \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \frac{F}{m_l} \end{bmatrix}$$

which results in an acceleration vector of $\mathbf{a} = (0, 0, 1.10)F/m_e$. It can be inferred that for an electron assigned to a valley which is transverse to the field direction, the acceleration vector would be $\mathbf{a} = (0, 0, F/m_t) = (0, 0, 5.26)F/m_e$.

Additionally, electrons may scatter against the lattice or an impurity and make an intervalley transition (known as intervalley (IV) scattering) [32]. We discuss the scattering of charges against the lattice and impurities in the next section.

2.1.3 Deformation Potential

Let us imagine the case of an electron with effective mass m^* propagating through a periodic potential U_L . A real crystal lattice does not remain static; it contains small deformations in its structure from an ambient, thermal phonon population or impurities which disrupt the periodic structure. The SuperCDMS detectors are composed of a high purity, semiconductor crystal that is held at millikelvin temperatures in its operation. In this regime, we expect that phonons which arise from zero-point fluctuations of the lattice are the dominant form of crystal deformations. These deformations in the lattice provide a potential U_S which induces charge-phonon scattering [4].

2.2 Charge-Phonon Scattering

Charge-phonon scattering describes two processes: the emission of a phonon and the absorption of a phonon both induced by a deformation potential as shown by the diagrams in Fig. 2.3. In both cases, we represent the wave-vector of the incoming electron with $\mathbf{k}$ and the wave-vector of the recoiling electron with $\mathbf{k}'$. The phonon, which is either emitted or absorbed, has a wave-vector $\mathbf{q}$ [4].

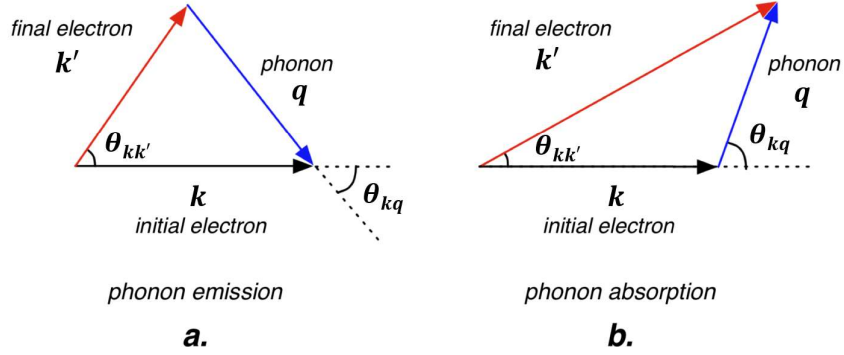


Figure 2.3: Illustration of two types charge-phonon interactions induced by a deformation potential. **a.** shows the emission of a phonon by an electron. **b.** shows the absorption of a phonon by an electron. Figure adapted from Fig. 2.9 in Ref. [4].

In the next sections, we explore the rate of both processes for an electron or hole as well as the kinematics which describe the interactions.

2.2.1 Interaction Rate

This section borrows heavily from Leman's [21] and Wang's [27] explanations.

We start by using Fermi's Golden Rule to calculate the interaction rate of the processes $\mathbf{k} \rightarrow \mathbf{k}' \pm \mathbf{q}$. The probability per unit time and per unit energy is given by

$$P_{k,k'\pm q} = \frac{2\pi V}{\hbar} |\langle \mathbf{k}' \pm \mathbf{q} | H | \mathbf{k} \rangle|^2 \delta(E_k - E_{k'} \mp E_q), \quad (2.16)$$

where H is the deformation potential Hamiltonian, V is the semiconductor volume, v_s is the longitudinal speed of sound in the medium, and E_k , $E_{k'}$, E_q is the energy of the initial electron, final electron, and phonon respectively.

We find that the amplitudes corresponding to the emission and absorption processes are

$$|\langle \mathbf{k}' + \mathbf{q} | H | \mathbf{k} \rangle|^2 = \frac{C^2 \hbar}{2V \rho v_s} |\mathbf{q}| (N_q + 1) \quad (2.17)$$

$$|\langle \mathbf{k}' - \mathbf{q} | H | \mathbf{k} \rangle|^2 = \frac{C^2 \hbar}{2V \rho v_s} |\mathbf{q}| N_q, \quad (2.18)$$

where C is the deformation potential constant, ρ is the material mass density, and the phonon occupation number is $N_q = 1/[\exp(\hbar v_s |\mathbf{q}| / (k_B T)) - 1]$

where k_B is the Boltzmann constant. Since the SuperCDMS detectors are held at sub-Kelvin operating temperatures, we find that $N_q|_{\hbar v_s|\mathbf{q}| \ll k_B T} \ll 1$. This limit yields a negligible charge-phonon absorption probability and the domination of charge-phonon scattering by the emission process.

The rate of emission can be found by integrating Eq. 2.16 over the phonon emission angle θ_{kq} and the recoil electron's energy $E_{k'}$. This yields an emission rate of

$$\frac{1}{\tau} = \frac{1}{3} \frac{v_s}{l_0} \frac{|\mathbf{k}|}{k_s} \left(1 - \frac{k_s}{|\mathbf{k}|}\right)^3, \quad (2.19)$$

where $l_0 = \frac{\pi \hbar^4 \rho}{2m^{*3}C^2}$ is the interaction length and $k_s = m^*v_s/\hbar$ is the wave-vector magnitude corresponding to the sound speed of the medium.

2.2.2 Charge-Phonon Scattering Kinematics

Before we move to the scattering kinematics, we transform to a momentum space in which the energy-momentum relationship is constant in every direction, known as the Herring and Vogt transform [33]. In this frame, we write the conservation of momentum

$$\hbar \mathbf{k} = \hbar \mathbf{k}' + \hbar \mathbf{q} \quad (2.20)$$

and conservation of energy

$$\frac{\hbar^2 |\mathbf{k}|^2}{2m^*} = \frac{\hbar^2 |\mathbf{k}'|^2}{2m^*} + \hbar v_s |\mathbf{q}|, \quad (2.21)$$

where $\mathbf{k}$ is the incoming charge wave-vector, $\mathbf{k}'$ is the charge recoil wave-vector, $\mathbf{q}$ is the phonon wave-vector, and v_s is the longitudinal speed of sound. We can then arrive to an expression for $|\mathbf{q}|$

$$|\mathbf{q}| = 2 \left(|\mathbf{k}| \cos \theta_{kq} - \frac{m^* v_s}{\hbar} \right), \quad (2.22)$$

where θ_{kq} is the emission angle of the phonon with respect to the direction of the incoming electron. The expression in Eq. 2.22 reveals two conditions that must be true for scattering to occur: the magnitude of the charge wave-vector $|\mathbf{k}|$ must be greater than the wave-vector magnitude corresponding to the sound speed of the medium $k_s = m^*v_s/\hbar$, the emission angle of the phonon must satisfy $\theta_{kq} \leq \pi/2$ [27].

The expression in Eq. 2.22 also allows us to rewrite $|\mathbf{k}'|$ as a function of the phonon emission angle θ_{kq} and the magnitude of the incoming wave-vector $|\mathbf{k}|$

$$|\mathbf{k}'| = \sqrt{|\mathbf{k}|^2 - 4k_s(|\mathbf{k}| \cos \theta_{kq} - k_s)} \quad (2.23)$$

We can then use the results from Eq. 2.22 and Eq. 2.23 to find the recoil angle of the charge in a similar manner

$$\cos \theta_{kk'} = \frac{|\mathbf{k}|}{2|\mathbf{k}'|} + \frac{|\mathbf{k}'|}{2|\mathbf{k}|} - \frac{2}{|\mathbf{k}||\mathbf{k}'|} (|\mathbf{k}| \cos \theta_{kq} - k_s)^2 \quad (2.24)$$

$$= \frac{|\mathbf{k}|^2 - 2k_s(|\mathbf{k}| \cos \theta_{kq} - k_s) - 2(|\mathbf{k}| \cos \theta_{kq} - k_s)^2}{|\mathbf{k}| \sqrt{|\mathbf{k}|^2 - 4k_s(|\mathbf{k}| \cos \theta_{kq} - k_s)}}, \quad (2.25)$$

where $\theta_{kk'}$ is the angle of the recoiling charge wave-vector $\mathbf{k}'$ with respect to the incoming charge wave-vector $\mathbf{k}$ and ranges from $0 \leq \theta_{kk'} \leq \pi$ for $k_s < |\mathbf{k}| < 2k_s$ and $0 \leq \theta_{kk'} \leq \pi/2$ for $|\mathbf{k}| > 2k_s$ [34].

2.2.3 Phonon Transport and Scattering

The three-dimensional wave equation of an emitted phonon is given by

$$\rho \omega^2 \epsilon_\mu = \sum_{\tau} \left(\sum_{\sigma \nu} c_{\mu \sigma \nu \tau} q_\sigma q_\nu \right) \epsilon_\tau, \quad (2.26)$$

where ρ is the mass-density of the crystal, ω is the angular frequency of the phonon, ϵ_μ is a component of its polarization vector $\boldsymbol{\epsilon}$, $c_{\mu \sigma \nu \tau}$ is the elastic tensor, and q_σ is a component of its wave-vector $\mathbf{q}$ [21]. Since $c_{\mu \sigma \nu \tau}$ is anisotropic, the group velocity

$$\mathbf{v}_g = \nabla_{\mathbf{q}} \omega(\mathbf{q}) \quad (2.27)$$

may not be oriented in the same direction as the quasi-momentum $\hbar \mathbf{q}$ which gives rise to the anisotropic transport and focusing of phonons in a crystal [16].

Phonons experience scattering from impurities (isotopic scattering) with a rate given in Eq. 2.28 as well as decay (anharmonic down-conversion) with a rate given in Eq. 2.29

$$\Gamma_I = A \nu^4 \quad (2.28)$$

$$\Gamma_A = B \nu^5, \quad (2.29)$$

where A and B are constants and ν is the phonon frequency [35].

In the next chapter, we explore how each of the physics processes mentioned in this chapter are modeled with a Monte Carlo simulation engine as well as the computational limits they impose.

Chapter 3

Monte Carlo Solution to Carrier and Phonon Physics

3.1 The Monte Carlo Method

In this section, we aim to describe the Monte Carlo approach to modeling charge and phonon transport which we will find necessitates the use of particle tracks. We then describe how tracking is done in Geant4 as well as how step sizes are selected.

3.1.1 Monte Carlo Approach to Particle Transport

The Monte Carlo approach to modeling physics processes such as charge transport involves modeling tracks which are updated by steps. Each step is subject to the probability of a physical processes occurring which limits the step size [19]. Stochastic number generation using probability distributions determines free flight duration and scattering events. Since the relevant charge transport process in cryogenic solid-state detectors is not homogeneous in position nor stationary in external forces or interaction rate, it becomes necessary to simulate individual carriers and track their dynamic histories to obtain the desired information [29].

3.1.2 Introduction to Tracking in Geant4

The current version of G4CMP and version of G4CMP used in this report¹ model the charge-phonon interactions as a single-scatter process. Since G4CMP is built on the base physics and machinery of Geant4, the charge and phonon tracking is done through `G4Steps`. At the start of each step, kinematic quantities such as position, momentum, and kinetic energy

¹G4CMP-V09-00-00



Figure 3.1: Illustration of a color-coded **G4Step**. The blue indicates the **AlongStep** section in which the continuous processes are modeled. The green indicates the **PostStep** in which kinematic changes from the production of secondaries are modeled. Figure adapted from Ref. [36].

are calculated. Along the step (**AlongStep**), continuous processes such as energy loss from ionization or energy gain from a field are simulated and combined with the end of the step (**PostStep**) decay processes which produce secondaries to update the track’s kinematic status. The step size is determined by the minimum of the following: the maximum allowed step length (user-defined) or the smallest step length provided by the physical interaction lengths of all associated processes [19]. G4CMP instead uses the **G4CMPTIMEStepper** routine to limit step sizes in free flight. This routine ensures that charge-phonon scattering occurs according to the interaction rate in Eq. 2.19 which has a strong dependence on energy and a threshold. In practice, the routine prevents a charge from gaining “too much” kinetic energy between interactions which in turn demands smaller step sizes at larger field values. Additionally, since an electron is subject to an effective mass that is dependent on the direction of its wave-vector, small steps become necessary to maintain the accuracy of the particle’s kinematic status [37]².

3.2 Carrier Physics

In this section, we verify that the charge carrier transport and scattering processes in G4CMP behave as theoretically predicted. We simulate a simple but artificial scenario: an electron or hole is placed in the center of an HVeV silicon detector and given 1 eV of kinetic energy. The charge is then allowed to propagate under 0 V or 4 V bias.

²Details regarding **G4CMPTIMEStepper** are undocumented at the time of this writing and are provided by the primary developer M.H. Kelsey, kelsey@slac.stanford.edu.

3.2.1 Carrier Trajectories

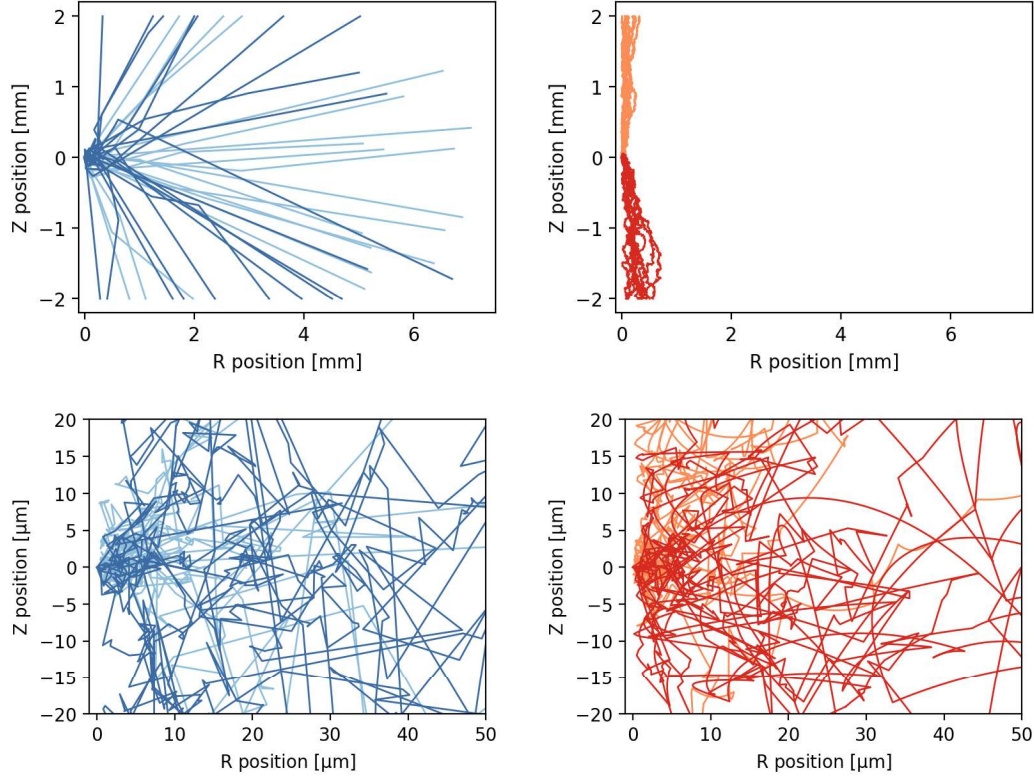


Figure 3.2: **Left:** Electron (light blue) and hole (dark blue) tracks under 0 V bias. **Right:** Electron (orange) and hole (red) tracks under 4 V bias. The top two figures display the full path length of charge tracks while the bottom half is a zoom-in on early interactions.

We start by observing the trajectories of a number of charge tracks at both bias settings, the result of which is shown in Fig. 3.2. Without a voltage bias, the charges begin their tracks with a wave-vector magnitude of $|\mathbf{k}| \approx 90 k_s$ for holes and $|\mathbf{k}| \approx 130 k_s$ for electrons. Combined with the straight trajectories between scatters, the large recoil scattering angles of the charges result in behavior that resembles a random walk. With each scatter, a phonon is emitted, and the charge loses kinetic energy, resulting in less frequent scatters according to the interaction rate Eq. 2.19. This leads to the below-threshold behavior in which the charges become ballistic and travel unimpeded to the detector surface.

Under 4 V bias, we observe similar scattering behavior to the 0 V case; larger scattering angles give the impression of a random walk at the start of each track. However, in the free flight duration between scatters, small steps taken during the `G4CMPTIMEStepper` trace out the trajectory of a charge drifting in the electric field. The electric field results in directed trajectories that give a net drift speed in the positive or negative Z -direction.

Additionally, along with the loss of kinetic energy due to the emission of phonons, the charge is continuously gaining kinetic energy from the electric field. This allows for the charge's wave-vector to remain above the k_s threshold and phonon emission to occur throughout the charge's entire trajectory to the surface.

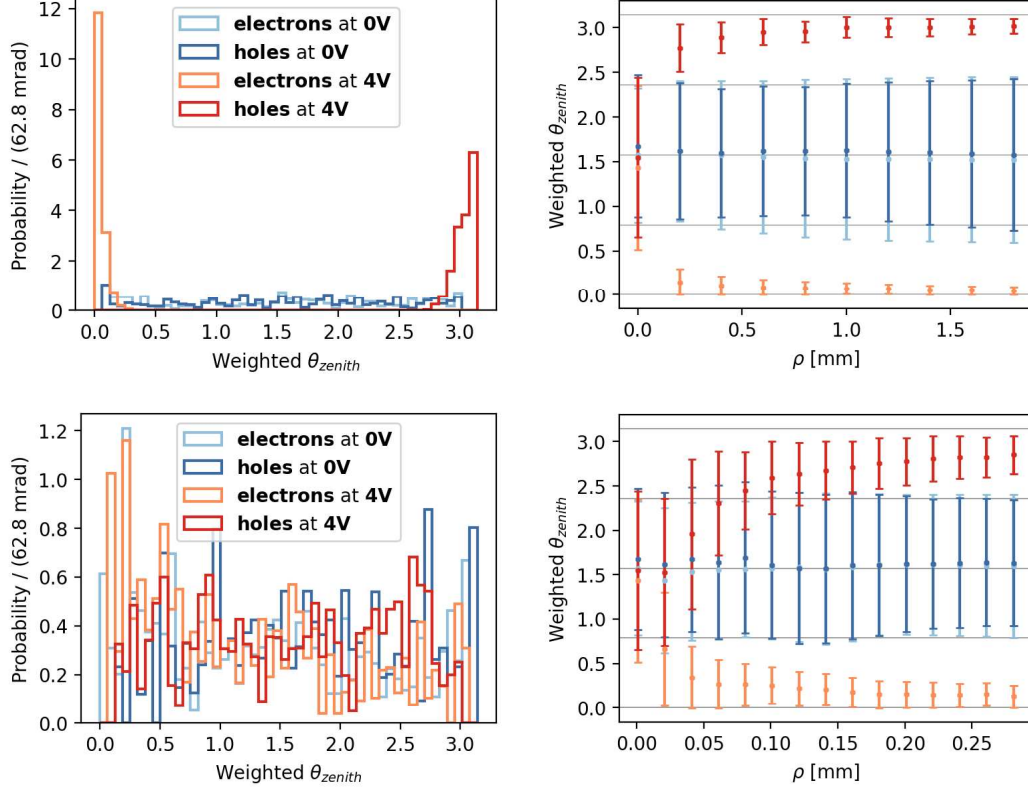


Figure 3.3: Illustration of randomness of charge trajectories as a function of distance from the origin ρ . **Left:** Example distribution of weighted zenith angle measurements at $\rho = 2$ mm (**Top**) and $\rho = 10$ μ m (**Bottom**) from the origin. **Right:** weighted zenith angle distributions as a function of distance from origin ρ for the full range (**Top**) and finer steps up to $\rho = 300$ μ m (**Bottom**).

We may also illustrate the random walk behavior of the charge trajectories as a function of distance from the origin using Fig. 3.3. We draw an imaginary spherical boundary around the origin with radius ρ . We then record the zenith angle θ_{zenith} at which the charge track passes through the boundary. The θ_{zenith} distribution is then weighted by a factor of $(2\pi R)^{-1}$ where $R = \sqrt{X^2 + Y^2} = \rho \sin \theta_{zenith}$ to remove the count bias which arises due to differing circumferences at different θ_{zenith} values.

The left two figures of Fig. 3.3 show the weighted θ_{zenith} distributions at $\rho = 2$ mm and $\rho = 10$ μ m. At $\rho = 2$ mm, we see that the distribution is largely flat for electrons and holes under no bias voltage while the electrons

and holes traveling under 4 V are traveling in the $\pm Z$ direction with more spread seen by the holes. In contrast, the weighted θ_{zenith} distributions at $\rho = 10 \mu\text{m}$ appear to be consistent for electrons and holes at either voltage, as in all cases, the carriers are interacting frequently with large scattering angles. There appears to be some slightly inflated probability for a weighted θ_{zenith} measurement at $\theta_{zenith} \approx 0$ or $\theta_{zenith} \approx \pi$ which is not yet understood.

The right two figures of Fig. 3.3 show the weighted θ_{zenith} distributions as a function of distance from the origin ρ . The top figure shows that while the electrons and holes under 0 V are consistently uniformly distributed, the electrons and holes under 4 V settle into their directed trajectories at $\rho \approx 250 \mu\text{m}$ from the origin. The bottom figure shows finer steps in ρ at a small distance which reveals the smooth transition from a random weighted θ_{zenith} distribution to directed trajectories under 4 V. The transition appears to occur earlier for electrons than holes.

3.2.2 Scattering Angles

In this section, we characterize the scattering angle $\theta_{kk'}$ between the incoming charge wave-vector $\mathbf{k}$ and the recoiling wave-vector $\mathbf{k}'$ after the emission of a phonon. A distribution of $\theta_{kk'}$ is shown in Fig. 3.4. It is seen that electrons and holes under 0 V or 4 V have distributions of scattering angles that are consistent with each other. The distribution is wide, covering the full $0 \leq \theta_{kk'} \leq \pi$ range, and peaks at $\theta_{kk'} \approx 1.8 \text{ rad}$. The large recoil scattering angles seen here are consistent with the random walk behavior seen in the previous section.

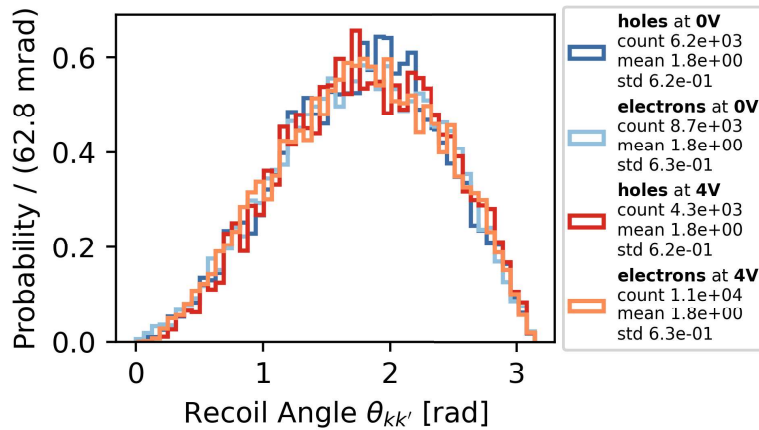


Figure 3.4: The distribution of scattering angles $\theta_{kk'}$ of the charge's recoil wave-vector $\mathbf{k}'$ with respect to its incoming wave-vector $\mathbf{k}$ using the inverse cosine of Eq. 2.24.

As we found with Eq. 2.24, if we look only at scatters in which $k_s < |\mathbf{k}| < 2k_s$, we find that the recoil angle $\theta_{kk'}$ distribution is restricted to $0 \leq \theta_{kk'} \leq \pi/2$. It is also seen that only the charge carriers under 0 V exist in this regime, as the electric field resulting from 4 V applied across 4 mm ($= 1 \text{ V/mm}$) provides the carriers with enough kinetic energy such that $|\mathbf{k}| > 2k_s$ always.

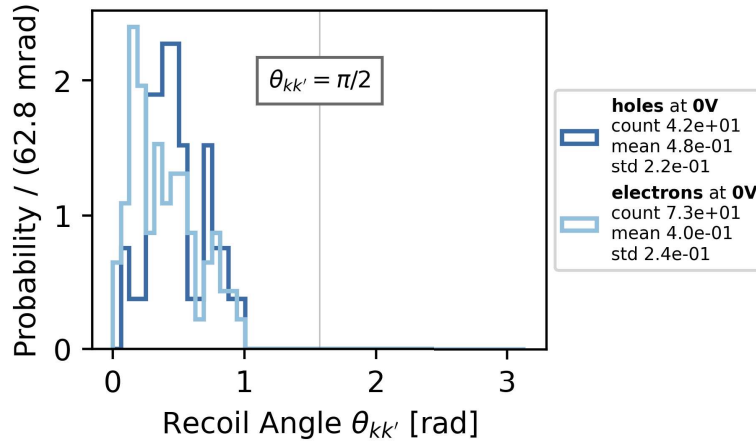


Figure 3.5: The distribution of scattering angles $\theta_{kk'}$ of the charge's recoil wave-vector $\mathbf{k}'$ with respect to its incoming wave-vector $\mathbf{k}$ using the inverse cosine of Eq. 2.24. This distribution is shown after a $|\mathbf{k}| < 2k_s$ cut is applied.

In the next section, we begin to look at the trajectories and scattering angles of the phonons emitted from charge-phonon interactions.

3.3 Phonon Physics

In this section, we use samples with the same configurations as Sec. 3.2. However, we will be looking at the tracks of the emitted phonons from charge-phonon interactions. We have configured the surfaces of the detector such that they absorb all phonons which interact with the boundary to avoid reflections. We also apply a cut to the phonon tracks to exclude tracks which originate from quasiparticle recombination in the aluminum fin of the QETs. With these modifications, we are able to focus only on the transport of phonons after their emission from charge-phonon scattering interactions.

3.3.1 Emission Angle

We start by checking the phonon emission angle θ_{kq} , or the angle between $\mathbf{k}$ and $\mathbf{q}$ shown in Fig. 3.6. We find that, again, the scattering angles of electrons and holes under 0 V or 4 V have distributions that are consistent with each other and cover the range $0 \leq \theta_{kq} \leq \pi/2$ as expected with a peak at $\theta_{kq} \approx 0.65$ rad.

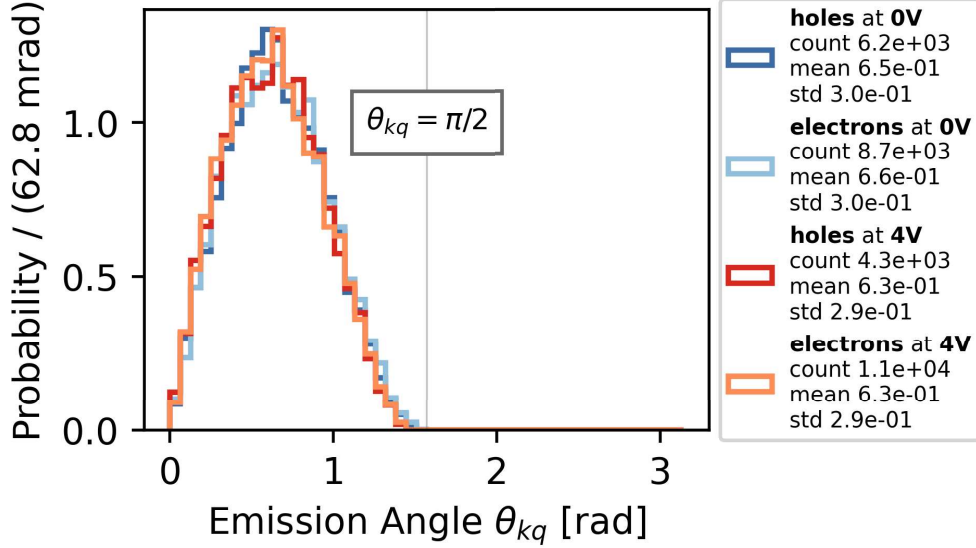


Figure 3.6: The distribution of scattering angles θ_{kq} of the phonon's wave-vector $\mathbf{q}$ with respect to the incoming wave-vector $\mathbf{k}$ of the charge. This quantity is provided by G4CMP's internal debug information.

We conclude that charge-phonon scatters are indeed forward-emitting for phonons. In the next section, we check the trajectories of phonons after their emission.

3.3.2 Isotopic Scattering and Down-conversion

We start with an evaluation of a phonon cascade resulting from a single charge-phonon scatter as shown in Fig. 3.7 where a total of 17 phonons were created and tracked until their absorption or decay. The parent phonon which is emitted from the scattering process begins its track with ~ 40 meV of energy and decays within ~ 4 ns to two phonons with energies ~ 27 meV and ~ 13 meV. As this process continues, each subsequent pair of created phonons have less energy and so less frequently scatter and downconvert according to Eq. 2.28 and Eq. 2.29. Qualitatively, we can verify the relationship between scattering frequency and energy, as the

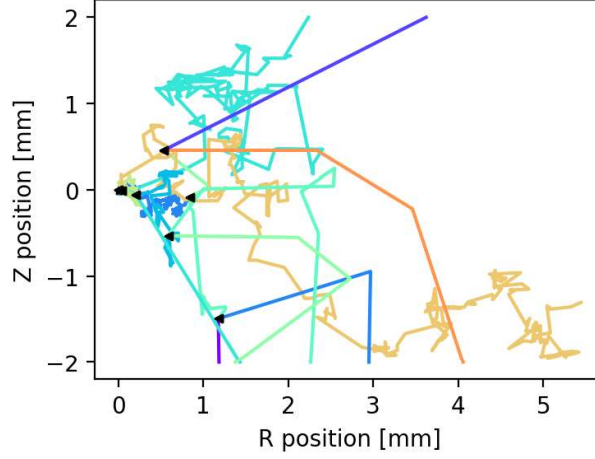


Figure 3.7: Cascade of phonons resulting from one charge-phonon interaction. Each phonon track is drawn with a unique color. The positions at which one phonon down-converts into two new phonons are marked with a black triangle.

last pairs of phonons which are created scatter just a few times over a relatively long distance before they are absorbed.

3.4 CPU Time for Different Processes

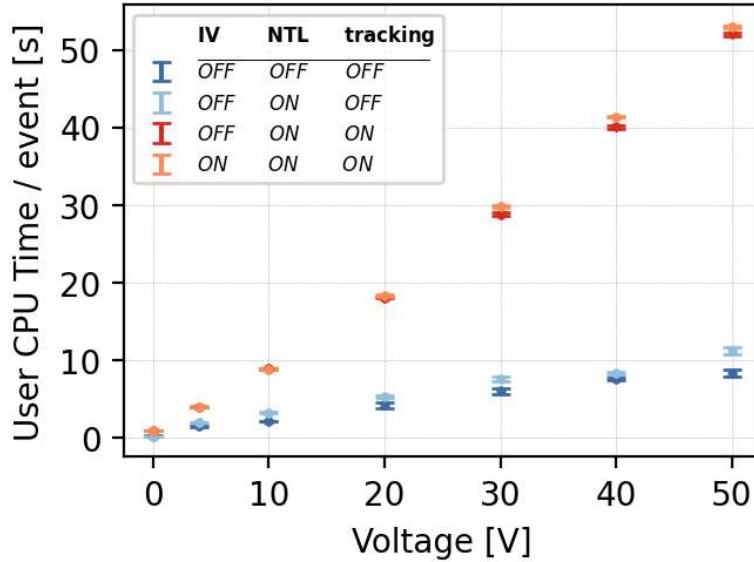


Figure 3.8: Relationship of user CPU time per event to detector voltage bias for single electron-hole pairs.

We start by establishing a baseline understanding of CPU time consumption for the interactions relevant to this investigation: charge and

phonon production, transportation, and scattering. The simulation is configured such that a 1.95 eV energy deposit occurs in the center of a SuperCDMS high-voltage eV-resolution (HVeV) silicon detector. For energies above the Si energy gap ($= 1.2 \text{ eV}$) but below the average energy per e^-/h^+ pair ($= 3.8 \text{ eV}$), only one e^-/h^+ pair is created [5]. The simulation can then be configured with different processes enabled for the single e^-/h^+ pair so as to determine where CPU time is consumed.

The results of this investigation are shown in Fig. 3.8. We find that in all cases, an increase in the detector's voltage bias increases the CPU time of the simulation. We find that the dependence on voltage bias comes from the `G4CMPTIMEStepper` routine which maintains smaller steps at higher field values.

The CPU time is observed to be minimized when all scattering processes are suppressed, allowing the charges to drift in the field (dark blue). When charge-phonon scattering (NTL) is enabled and the tracking of emitted phonons is suppressed (light blue), there is an increase (up to $\sim 150\%$) in CPU time, as the path length of the charges is increased by interactions which modify their trajectory, increasing the number of steps taken before a charge reaches a detector surface. The most noticeable change is seen once the emitted phonons are tracked (dark red) which increases the CPU time by a factor of ~ 5 . Lastly, for completeness, we enable intervalley scattering along with the previously mentioned processes (orange) to find that its impact is small ($\sim \text{few } \%$).

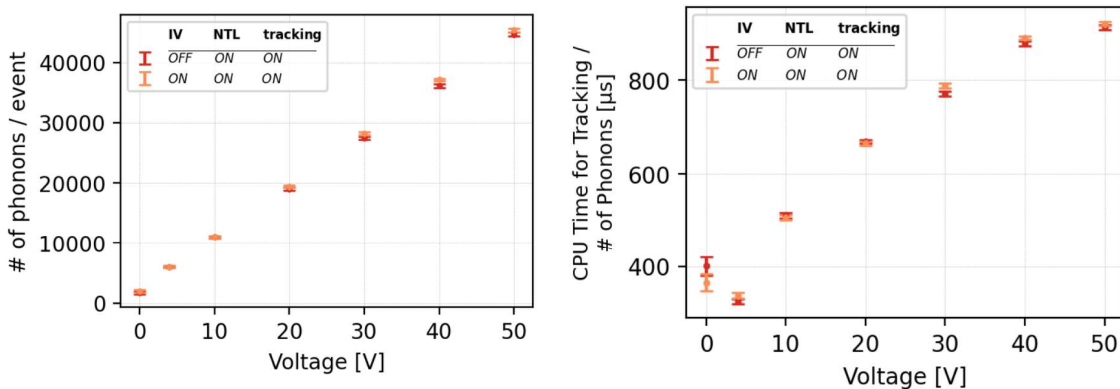


Figure 3.9: **Left:** Relationship of phonons per event to detector voltage bias for single electron-hole pairs. **Right:** Ratio between the CPU time increase for phonon tracking and the number of phonons as a function of voltage.

We now would like to understand where the CPU time consumption comes from, as it was the tracking of emitted phonons that was the largest contributor as seen in Fig. 3.8. We saw in the previous section that a single

charge-phonon interaction can result in a cascade of multiple phonons. The results of Fig. 3.9 show what appears to be a similar linear relationship between the number of phonons and the detector bias voltage as Fig. 3.8. However, the right of Fig. 3.9 shows that the ratio of the CPU time increase for phonon tracking (light blue subtracted from red and orange in Fig. 3.8) to the number of phonons (left of Fig. 3.9) is not constant as a function of voltage. This suggests that the number of phonons tracked does not have a direct relationship with CPU time.

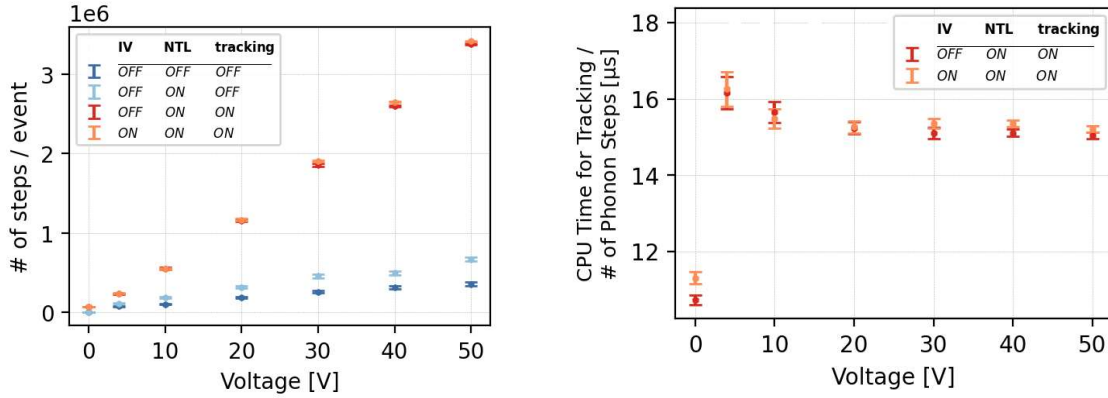


Figure 3.10: **Left:** Relationship of steps taken per event to detector voltage bias for single electron-hole pairs. **Right:** Ratio between the CPU time increase for phonon tracking and the number of phonon steps as a function of voltage.

We then turn to looking at the number of steps taken per event as a function of voltage, shown in the left of Fig. 3.10. Repeating the previous method results in the right of Fig. 3.10. This figure shows that the ratio of the CPU time increase for phonon tracking (light blue subtracted from red and orange in Fig. 3.8) to the number of steps taken by phonons (light blue subtracted from red and orange in left of Fig. 3.10) which is a constant function of voltage: $\sim 15 \mu\text{s}/\text{step}$. This suggests that the number of steps taken by phonons does have a direct and linear relationship with CPU time.

This result is in agreement with the findings in Sec. 3.3.2 as well as Eq. 2.28 and Eq. 2.29. The range of energy of phonons emitted from charge-phonon interactions is expected to scale with the detector voltage bias which does work on the charge carriers, increasing their mean energy [4]. The higher-energy phonons produced under a voltage bias are then expected to scatter and decay more frequently, increasing the overall number of steps. The number of phonons produced, alone, is thus not the only contributing factor to the increase in CPU time.

3.5 Conclusions

This section summarizes the main takeaways from the work conducted this summer to investigate the way that charge carrier and phonon physics processes are modeled in G4CMP. It also describes what future work may entail considering the findings shown in this report.

3.5.1 Summary of the Problem at Hand

The purpose of Chapter 3 was to both establish an understanding of which physics processes consume the most CPU time and validate that the physics processes provide the expected results according to Chapter 2.

We validated that the charge transport and scattering is behaving as expected with regard to the interaction rate (Eq. 2.19) and scattering angles (Eq. 2.24). We noted that a remarkable result of the large range of recoil scattering angles from charge-phonon interactions is that the tracks appear similar to a random walk when scattering is frequent.

We have shown that the emission angle distribution of phonons produced from the charge-phonon interactions is limited to $\theta_{kq} \leq \pi/2$ as expected. An investigation into the way the cascade of phonons resulting from a charge-phonon interaction is modeled qualitatively validates the scattering (Eq. 2.28) and down-conversion (Eq. 2.29) rates.

We established that while CPU time generally has a direct relationship with the detector bias voltage, the phonon tracking process is the most costly due to the sheer number of phonon steps.

3.5.2 Future Work

Future work includes further verification that the number of phonon steps is directly responsible for the increase in CPU time. This may be in the

form of running a profile on G4CMP.

Once the source of the slow-down is confirmed, it may prove to be beneficial to migrate away from a single-scatter model for charge carriers and/or phonons. A candidate model may be multiple scattering theory which allows the Monte Carlo simulation to take coarser steps while approximating the particle’s final angle distribution and displacement resulting from processes which occurred during the step [38]. The usual practice is to use models described by either Molière [39, 40], Goudsmit & Saunderson [41, 42], or Lewis [43], the physical assumptions of which are shown in Table 3.1 [38].

Model	Small scattering angle	Negligible energy loss
Molière	Yes	Yes
Goudsmit & Saunderson	No	Yes
Lewis	No	No

Table 3.1: Summary of physical assumptions for the multiple scattering models: Molière, Goudsmit & Saunderson, and Lewis.

Molière’s theory relies on a high-energy, small-angle approximation to model the “soft” scatters of high-energy particles through a geometry. Goudsmit & Saunderson and Lewis allow for large scattering angles from “hard” scatters through the expansion of Legendre polynomials. Molière and Goudsmit & Saunderson assume that the energy loss within a step is negligible while Lewis makes the continuous slowing down approximation to account for energy loss [38]. Considering the results we found in the previous section, the Lewis model may be most appropriate as a starting point. We saw that the scattering angles of charges and phonons are large enough that a small-angle approximation would prove to be an inaccurate model. Additionally, the energy loss from charges emitting a phonon or from the down-conversion of a phonon into two lower-energy phonons is non-negligible.

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