

# Semiconductor phonon and charge transport Monte Carlo simulation using Geant4

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*Keywords:*

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1.

## 2. Introduction

In this paper we present a Monte Carlo simulation of phonon and charge transport in Semiconductor crystals using Geant4. Geant4 is a sophisticated C++ based Monte Carlo simulation toolkit maintained by an international collaboration. The toolkit was originally developed in support of High Energy Physics (HEP) experiments. It provides functionality for the simulation of the passage of particles through complex detector geometries and aims to accurately simulate all interactions of the particles with the matter through which they pass. Today, the Geant4 toolkit is an important tool both for HEP particle accelerator based experiments building Detector Monte Carlo(DMC) simulations as well as any experiment wishing to estimate backgrounds from environmental or cosmic ray radiation source.

This paper documents our effort to build a cohesive Geant4 Condensed Matter Physics Monte Carlo simulation toolkit, G4CMP. This effort is motivated by the Cryogenic Dark Matter Search (CDMS) dark matter direct detection experiment. The CDMS detectors are cylindrical Germanium crystals of approximate size  $75\text{mm} \times 25\text{mm}$ , cooled to  $60\text{mK}$ . Dark matter particles may recoil from Ge nuclei via the weak force and thus create phonons and free electron-hole pairs within the crystal. Electron-hole pairs are collected at the crystal surface by a small ( $\text{V/cm}$ ) drift field. Phonons are detected by Transition Edge Sensor (TES) bolometers. The need for an accurate Detector MonteCarlo simulation of the CDMS detector has provided the chief motivation for the work described in this paper.

The phonon and charge transport code described here attempts to accurately model all physics processes believed to be relevant to phonon and

charge collection at cryogenic temperatures. This includes anisotropic phonon transport/phonon focusing, phonon isotope scattering, anharmonic downconversion, oblique carrier propagation and emission of Luke-Neganov phonons by accelerated carriers. We believe that the resulting G4CMP framework is sufficiently general that it can be useful to other experiments employing cryogenically cold charge or phonon detectors.

### 3. Phonon Transport

Phonon transport was the first component of the G4CMP framework to be developed and early results were presented at LTD-14. Since the phonon transport code described here is intended for temperatures  $T < 1\text{K}$ , scattering off thermally excited background phonons is ignored. Currently, only acoustic phonons are simulated.

#### 3.1. Anisotropic transport and phonon focusing

Phonons are quantized vibrations of the crystal lattice. The propagation of phonons is governed by the three-dimensional wave equation [? ]:

$$\rho\omega^2 e_i = C_{ijlm} k_j k_m e_l \quad (1)$$

where  $\rho$  is the crystal mass density,  $\omega$  is the phonon frequency,  $\vec{e}$  is the polarization vector,  $\vec{k}$  is the wave vector and  $\vec{C}_{ijml}$  is the elasticity tensor.

For any given wave vector  $\vec{k}$  Equation 1 has three eigenvalues  $\omega$  and three eigenvectors  $\vec{e}$ . These correspond to the three different polarization states *Fast Transverse (FT)*, *Slow Transverse (ST)* and *Longitudinal (L)*. The actual direction and velocity of propagation of phonons is given by the group velocity vector  $\vec{v}_g = d\omega/dk$ . The group velocity can be calculated by interpreting  $\omega$  in Equation eq:3DWave as a function of  $\vec{k}$ :

$$\vec{v}_g = \frac{d\omega(\vec{k})}{d\vec{k}} = \nabla_{\vec{k}}\omega(\vec{k}) \quad (2)$$

Due to the anisotropy in  $C_{ijlm}$ , Eq. eq:GroupV yields a group velocity  $\vec{v}_g$  which is not parallel to the phonon momentum  $\hbar\vec{k}$ . Instead, phonons are focused onto propagation directions which correspond to the highest density of eigenvectors  $\vec{k}$ . This focusing gives rise to intensity caustics when observing the energy intensity distribution resulting from a point like phonon source isotropic in  $\vec{k}$ -space. The resulting caustics can be observed using

microcalorimeters [cite XXX]. It can be seen from Figure [XXX] that the caustics simulated by the Geant4 phonon transport code are in good agreement with experimental observations.

For the purposes of the G4CMP phonon transport code, the wave equation is not solved in real time but rather a look-up table is generated which maps  $\vec{k}$  onto  $\vec{v}_g$ . Bilinear interpolation is used to generate a continuous mapping function. Phonon focusing and methods for solving the three-dimensional wave equations are treated in great detail in [cite XXXX].

### 3.2. Phonon processes

In addition to the phonon equation of motion, which is given by the three dimensional wave equation Eq.eq:3DWave, two processes are relevant to acoustic phonon transport in cryogenic crystals: Isotope scattering and anharmonic down conversion. The scattering and downconversion rates for phonons in the cryogenic crystal are given by

$$\Gamma_{scatter} = B\nu^4 \quad (3)$$

$$\Gamma_{anh} = A\nu^5 \quad (4)$$

where  $\Gamma_{scatter}$  is the number of scattering events per unit time,  $\Gamma_{anh}$  is the number of anharmonic downconversion events per unit time,  $\nu$  is the phonon frequency and  $A$ ,  $B$  are constants of proportionality derived from the elasticity tensor [cite XXXX].

The isotope scattering process occurs when a phonon interacts with an isotopic substitution site in the lattice. It is effectively an elastic scattering process during which we assume the phonon momentum vector to be randomized. During this scattering process the phonon polarization state can change freely between the three states  $L$ ,  $ST$ ,  $FT$ . The branching ratio between the three polarizations is determined by the relative density of allowed states for each polarization. This change between polarization states is often referred to as mode mixing.

The anharmonic down conversion process causes a single energetic phonon to decay into two phonons of reduced energy. In the simulation, this process conserves energy but not momentum, since momentum is exchanged with the crystal lattice. While in theory all three polarization states can decay, the downconversion rate of  $L$ -phonons completely dominates the energy evolution

of the phonon system [cite XXXX], with downconversion events from other polarization states being negligible.

-Cryo: No scattering -Current: Acoustic only -Focusing: Achieved by mapping (from elasticity tensor) and bilinear interpolation -FIGURE::Focusing validation

-Phonon processes: -Constants from Elasticity tensor -Isotope scattering and mode mixing -Anharmonic down conversion -Quasi-diffuse propagation

#### **4. Charge Transport**

#### **5. Conclusion**