Carrier transport and phonon emission in germanium detectors of the cryogenic dark matter search

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Abstract. The Cryogenic Dark Matter Search (CDMS) measures both the ionized charge and the energy in athermal phonons created by particle interactions in ultrapure Ge and Si crystals at a temperature of 40 mK. Charge collection potentials must remain at only a few volts, else emitted phonons from drifted carriers will dominate the phonons of the original interaction. In this regime, there are practically no thermal phonons and carrier transport is determined by phonon emission. We present results for drift-limited carrier dynamics and rates of phonon emission. As these transport conditions represent an extreme limit, a Monte Carlo technique was used to bypass analytical assumptions commonly used in solving the Boltzmann transport equation. This work will assist us in understanding phenomena found in our detectors.

1. Introduction
CDMS seeks to detect the scattering on Ge and Si crystals of putative weakly-interacting massive particles (WIMPs) which could form the dark halo of our galaxy. Ionization and phonon signals are measured simultaneously, allowing us to distinguish between electron and nucleon recoils. This measurement technique provides discrimination between the expected signal of WIMPs and electromagnetic background. These detectors are cylindrical in geometry, 1 cm thick and 3.81 cm in radius. One cylindrical face is metalized into geometries forming electrodes. These electrodes are voltage-biased (-3V Ge, -4V Si) and collect ionization from recoil events. The opposite cylindrical face measures a thermal phonon flux. It is divided into quadrants each of 1036 Al phonon collection fins coupled to W transition-edge sensors. This face serves also as a ground potential for ionization collection. Carrier-phonon interaction affects both our phonon and ionization measurements, so it is critical to understand the fundamental mechanisms of carrier-drift dynamics under our particular operating conditions.

This work examines carrier transport in our germanium detectors. Our germanium crystals are metalized in the direction of <100> with impurity concentrations of a few $10^{10}$ cm$^{-3}$. Drift fields of 3 V/cm at a temperature of 40 mK are conditions not standard in the literature.

We report on the results of a Monte Carlo simulation based on the wealth of literature on carrier transport in semiconductors [1-7]. We are able to predict the emission of phonons by carriers (the Luke-Neganov effect), as well as the carrier energy and spatial distribution functions. This allows us to compute properties such as mobility, diffusion, and carrier-trapping probabilities.
2. Background and simulation techniques
In our transport regime, the number of thermal phonons is negligible for the drift fields of interest. Carrier scattering is dominated by spontaneous phonon emission (or collision with zero-point fluctuations of the lattice), often called the "zero-point" regime. It is often considered in the literature [1-4] that germanium mobility data at 8 Kelvin is representative of zero-point behavior. Our operational temperature is two magnitudes lower than this value. With our small drift fields, it has been an open question how representative the 8 Kelvin data are of our conditions.

This Monte Carlo simulation follows closely that of [1][5]. Scattering probability rates, derived from Fermi's Golden Rule, are numerically computed beforehand and are implemented as a function of energy. The simulation propagates a carrier in a uniform electric field. The step size is chosen such that the carrier has only a small probability to scatter, and are usually just accelerated by the field. A small proportion of the time, they scatter via one of the allowed mechanisms. Once this occurs, the carrier is reoriented with the appropriate random distribution for the given scattering mechanism. The momentum vector is rescaled for appropriate energy and momentum conservation. The carrier is propagated in this way, long enough to be well-equilibrated in these conditions. The final position, momenta, and scattering history of the carrier are recorded, and the simulation is repeated to produce an ensemble of many such carriers.

3. Electrons
We are drifting carriers in the <100> direction, yet the principal axes of the eight L half-valleys are oriented in the permutations of <111>. As this does not kinematically favor any particular valley along the electric field, by symmetry a spherical treatment of the electrons should be adequate. Nonparabolicity was considered in the calculation of scattering rates, and in incrementing position and momentum. Emission and absorption rates for phonon scattering are calculated for acoustic, intervalley, and optical processes. The scattering rates for electrons were calculated through a density of states formulation. The choice of a final momentum state does consider inelasticity, but as yet assumes that electron scattering is isotropic. We are in the process of introducing the full anisotropy found in choosing the final state, which is due to the dependency on the density of available momentum states combined with the elliptical nature of the valleys.

4. Holes
Holes spend only a few percent of the time occupying the light band before decaying to the lower-energy heavy band. Consequently, it is common to neglect all but the heavy band. In this simulation, both bands are considered in a parabolic way. In a manner similar to [7], this requires four independent scattering rates (intraband and interband) for each phonon scattering process.

Warped bands have been accounted for. A direction-dependent effective mass is used to increment position and velocity. Similar to [7], wavefunction overlap integrals are included in calculating scattering rates, and in selection of a final k-state. This makes final-state selection somewhat more complicated than the electron case. A random number search using a rejection technique is employed to select a suitable magnitude of phonon wavevector, \( q \). Final values for electron wavevector and scattering angle are then constrained by energy and momentum conservation.

Some common assumptions and approximations have been re-examined in order to accommodate our extreme low-temperature, low-bias case. Unlike assumptions in previous work [1,2,4], there is no approximation of near-elastic energy conservation for phonon magnitudes. Available scattering angles are defined explicitly and series-expansions are not used to satisfy energy conservation.
Figure 1. A comparison of electrons and holes, $8 \, K$ (diamonds) and $40 \, mK$ (squares). Top graphs show drift velocity compared to pre-existing $8 \, K$ theory (continuous lines) and experiment (points) [1-4]. Data from [8] denoted as *. The next two rows of graphs show simulated diffusion, longitudinal and transverse. The bottom row shows the ratio of energy dissipated by acoustic phonon emission to that of all phonon emission processes.

5. Findings

Although we did not use this as input, simulated drift velocities for $40 \, mK$, $0.5 \, V/cm$ are found to match well to those experimentally measured at $T=20 \, mK$, $E = 0.5 \, V/cm$ (holes: $v_d = 1.67 \times 10^6 \, cm/s$, electrons: $v_d = 2.37 \times 10^6 \, cm/s$) as reported by [8].

For electrons, simulated drift velocities at $8 \, K$ match well to data and to prior simulation as in [1-4]. See figure 1. As pointed out in [1], it is known that the data for Ge $<111>$ electron velocities depict a negative differential resistance, which causes velocity to diverge from that of the $<100>$ direction at about $2 \, V/cm$. Our $<100>$ simulated electron velocities replicate well the existing $<100>$ theory. By simulating $T = 40 \, mK$, we find that $8 \, K$ is not well represented by the zero-point approximation for
electrons at our bias levels. A factor of 2-3 increase in electron drift velocity is seen for fields of a few $V/cm$. At this lower temperature, both diffusion constants also increase for electrons. Previous work [1-4] on hole simulation did not match well to data in the low-temperature/low-field range. With these results, we see that simulation matches well to data, and that there is generally little difference upon comparing $8 \text{ K}$ to $40 \text{ mK}$. Although heavy, holes have high carrier energies relative to electrons due to lower scattering rates. Substantial emission of optical phonons by holes at fields only of the order $V/cm$ was not anticipated. Consequently, the pronounced maxima in the diffusion of holes seen in figure 1 may not have been previously investigated. At field-strengths higher than about $10 \text{ V/cm}$, hole mobility begins to decrease due to the onset of substantial optical phonon emission.

Comparing the energy histograms of carriers under drift (figure 2) gives some indication of processes likely to occur in bulk germanium. The scattering rate of holes is less than that of electrons because of differences in deformation potentials and the effect of warped valence bands. Consequently, holes reach a drift-limited equilibrium at energies substantially higher than electrons. The binding energy of hydrogenic impurities in germanium is only $12 \text{ meV}$, which makes it likely that holes impact ionize such levels. The threshold for optical phonon emission is $37 \text{ meV}$, which holes readily exceed and soon scatter to low energies through the emission process.

![Figure 2](image_url)  
Figure 2. The normalized energy distributions of electrons and holes under drift.

6. Conclusions
We have been able to reproduce the theoretical and experimental results obtained for electrons at low temperature and low field, and to fix the problems existing in the literature with holes. While electron transport is dominated by the emission of acoustic phonons, holes appear to emit a substantial amount of optical phonons. This model has to be validated further with the measurements of drift velocities at low field at $40 \text{ mK}$ that we are currently performing.

This Monte Carlo simulation will be a valuable tool to understand better the behaviour of detectors, in particular carrier trapping on neutral and ionized impurities, and the energy and angular distribution of the Luke-Neganov phonons emitted by the carriers. Such phonons modify the rise time of our phonon pulses, which is a principal discrimination tool against surface electrons.

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