Phonons and Charge Carriers in Crystals

Michael H. Kelsey
SLAC GEANT4 Group

GEANT4 Collaboration Meeting
29 Sep 2015

Outline

- Introduction
- G4CMP Library Features
- Phonon Physics
- Charge Carrier Physics
- Development Plans

Introduction

CDMS experiment uses MATLAB simulation for phonon and charge carrier propagation through cryogenic (50 mK) germanium detectors

- Geant4 simulation of backgrounds (neutrons, gammas)
- Record energy deposition (hits) to text file
- Text file input to MATLAB, parametrize $E \to N_{\mathrm{phonon}}$
- Desire to integrate detector response into G4 simulation

Development of phonon physics in G4 started in 2009, extended example

Mods to tracks (group velocity like optical photons), crystal parameters in container class included in toolkit (10.0)

G4CMP External Library

Phonon physics included in extended/exoticphysics/phonon

Further development, including charge carrier physics, done outside Geant4, in a SLAC-CDMS Git repository

- External library, linked with user's application *before* G4
- Includes physics processes, support classes
- Crystal-structure container supersedes G4 toolkit version

D. Brandt (SLAC), M. Kelsey (SLAC), P. Redl (Stanford), R. Agnese (FSU)

G4CMP Features

Expanded version of **G4Lattice** parameter container

Electric field class to handle 4D mesh fields (e.g., COMSOL)

Equation of motion handles mass tensor, valley propagation

Process to convert energy deposition from “regular” particles to phonons, electron-hole pairs

GNUmake, CMake support for building, linking

G4Lattice Extensions

G4 toolkit `G4LatticeLogical` has only phonon parameters

- Dynamical constants $\beta, \gamma, \lambda, \mu$
- Scattering constant b, decay constant a
- Densities of states for phonon polarizations
- Lookup tables for group velocities

Additional parameters for charge carrier propagation

- Sound speed
- Scattering lengths for electrons and holes
- Mass tensor and scalar mass values
- Valley directions
- Field scale, rate and exponent for intervalley scattering

Member functions for phonon, charge carrier kinematics (momentum, velocity, wavevector, Herring-Vogt coordinates)

Phonon Physics

Phonons are collective oscillations of crystal lattice

- At low temperatures, *acoustic* phonons propagate with either transverse or longitudinal oscillations
- At higher temperatures, in crystals with larger unit cells (more than one net atom), *optical* phonons propagate with the unit cell out of phase
- G4CMP only treats acoustic phonons, cubic lattices

Three types for phonons: longitudinal, "slow" and "fast" transverse

- Different $v_g - k$ relations, scattering processes
- Different `G4ParticleDefinition` types ease distinctions

Phonon Physics

Minimal number of processes implemented

Scattering

Direction and polarization change due to scattering off lattice impurities or defects

Downconversion

Longitudinal phonon can convert to lower energy pair

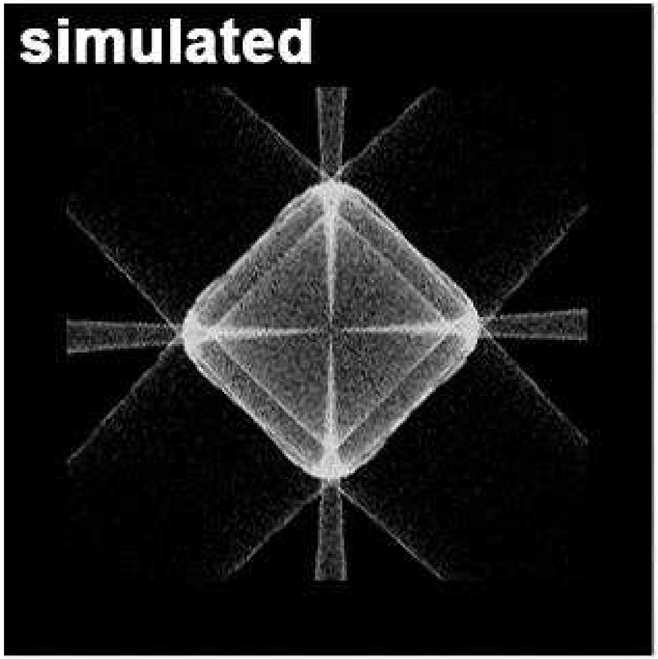
$L \to L'T$ or $L \to TT$

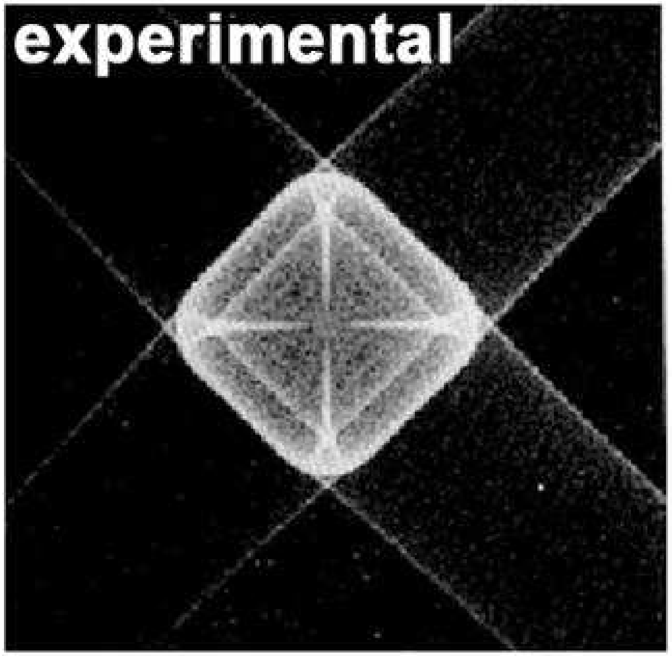
Reflection

Very simple, just specular reflection at boundary

Reflection needs major expansion to properly treat group velocity, critical angles, refraction/transmission, etc.

Phonon Physics





G4CMP simulation of Ge cube with point phonon source on face

Phonon hits recorded on opposite face

Caustics show focussing of trajectories along preferred crystal axes

Experimental data with heat pulse (laser hit) on face of Ge cube

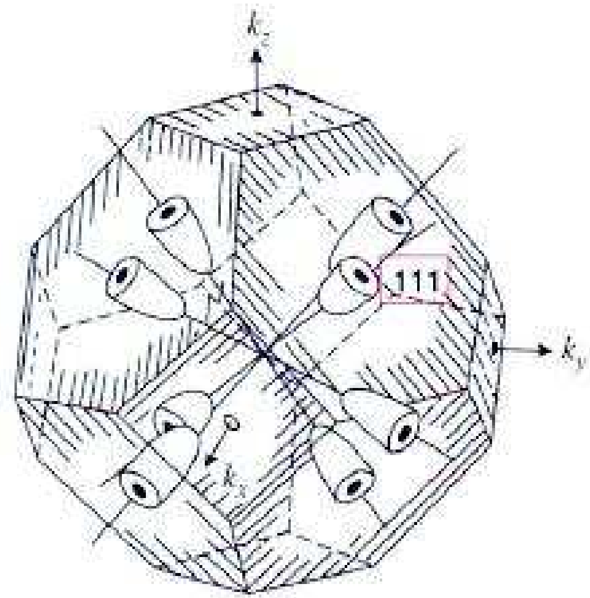
Phonons recorded on opposite face

Northrop and Wolfe, PRL **19** *1424 (1979)*

Phonon Physics

Movie singlePhonon.mpeg here

Charge Carrier Physics



L valleys of Ge

Electrons and holes propagate in crystal with *effective masses*

In general, depends on orientation of momentum w.r.t. lattice (Brillouin zone valleys): **mass tensor**

Currently, only electrons have mass tensor (for germanium); holes have scalar mass

Charge Carrier Physics

Electrons and holes have special `G4ParticleDefinition` (i.e., not `G4Electron`)

Static lookup table keeps track of which valley electron is in

Kinematics handled by special equation-of-motion class, tied to E-field

Utility class (`G4LatticePhysical`) maps electron momentum to other quantities (energy, velocity) via mass tensor, valley

Charge Carrier Physics

Several physics processes, with shared base classes and electron-hole specializations

Luke phonons

Emit phonons via Luke-Neganov process (analogous to Cherenkov photons): threshold at velocity equal to sound speed, rate increases with energy

Intervalley scattering

Transfer from one Brillouin valley to another without change in momentum vector

TimeStepper

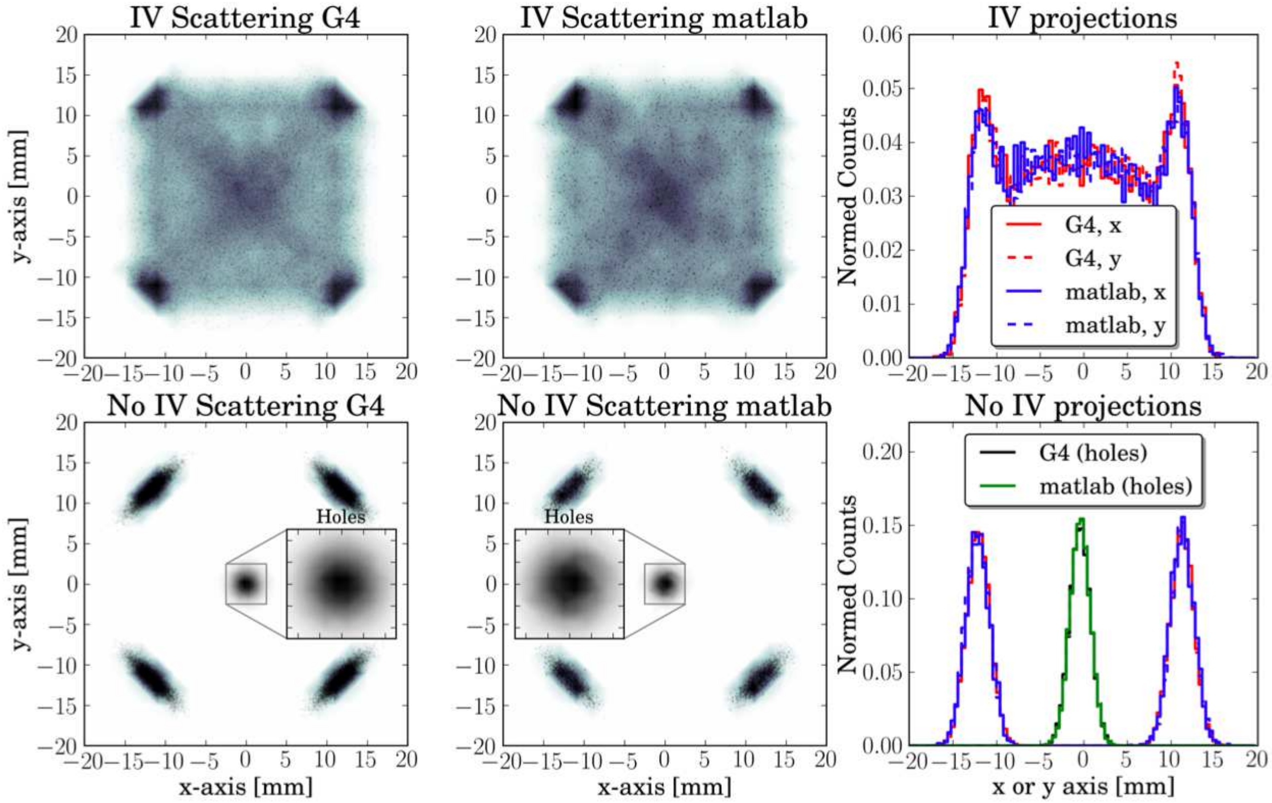
Step-limiting process, ensures charge carriers don't gain too much energy before generating phonons

Charge Carrier Physics

Movie e-hole_movie.mpeg here

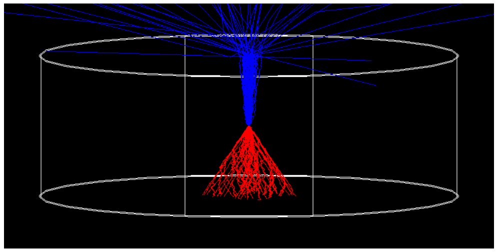
Charge Carrier Physics

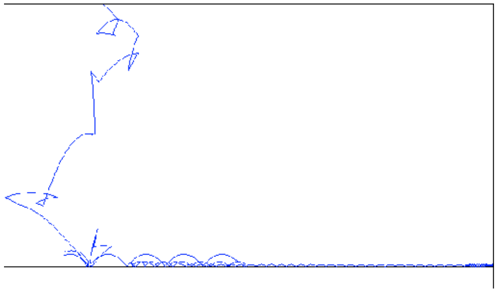
Comparison of G4CMP with SuperCDMS Matlab-based Simulation



Propagation of electrons and holes through 25 mm Ge crystal with 4 V along z direction, with and without intervalley scattering

Open Issues





Small step size problems during boundary reflection

- "Pass through" boundary into next volume
- Get stuck at boundary
- "Bounce" along boundary many times

Phonons need to transfer energy to volumes in contact at boundary (e.g., for TES detectors)

Support more than just germanium (provide parameter files, tools to compute parameters from lattice constants)

Development Plans

Implement proper phonon boundary process, reflections with $v_g - k$ misalignment, transmission at crystal-crystal boundaries, etc.

Replace TimeStepper with better handling of thresholds and limits for charge-carrier processes

Integrate tools for generating $v_g - k$ lookup tables

Document, provide tools for calculating parameters

Move development out of SLAC CDMS space?