Cryogenic Device Simulation with G4CMP

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Radiation Impact on Superconducting Qubits
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Motivation

There is a strong experimental connection between the effect of radiation, and the response of semiconductor devices to that radiation.

Whether for radiation monitoring, rare-event experiments, or quantum computing devices, simulation is important for detector design and for understanding backgrounds and signals.

Having a reliable simulation of the entire detector chain – from Geant4 radiation, through energy distribution in a device, to modelling readout – would be useful to many communities.

G4CMP provides a library integrated with Geant4 particle tracking and processes, so you can run that whole simulation chain in a single job.

Outline

- Overview of G4CMP Features
  - Defining Crystal Properties ("Lattice Configuration")
  - Phonon Transport and Interactions
  - Charge Transport and Interactions
  - Electric Field Modeling, Sensor Response
- Near-term Development Work
- Software Access

Many details of individual processes included in backup slides and our 2023 publication

G4CMP : Condensed Matter Physics for Geant4

Transport of **meV-scale** (acoustic) **phonons** in deeply cryogenic crystals

- Mode-specific relationship between wavevector and group velocity
- Impurity scattering (mode mixing), anharmonic decays

Transport of **eV-scale** (conduction band) **electrons** and **holes** in crystals

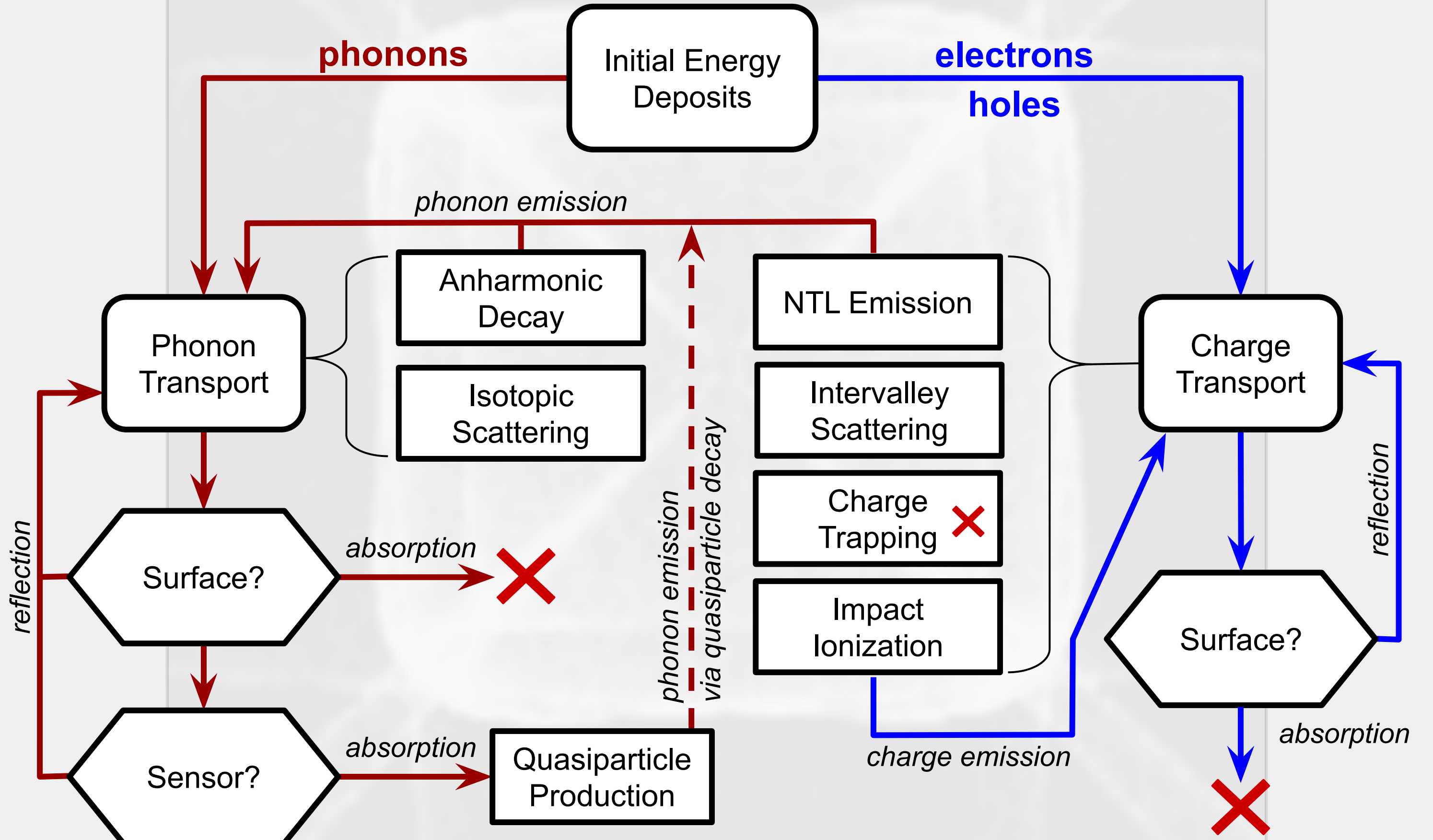
- Anisotropic transport of electrons, including electric field effects
- Scattering, phonon emission (NTL), trapping

Production of electron/hole pairs and phonons from energy deposits

Utility classes to support detector response

- Finite-element mesh electric fields (2D and 3D)
- Phonon absorption, detection in superconducting films

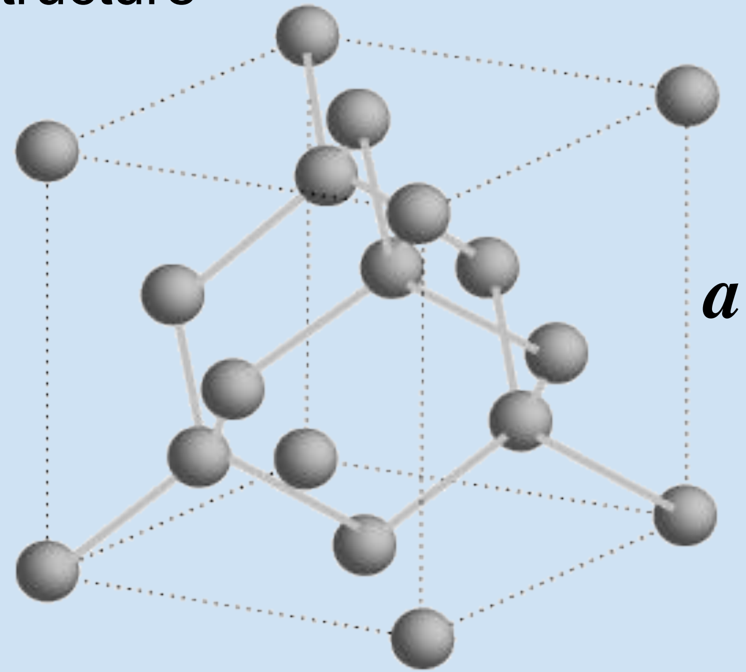
G4CMP : Condensed Matter Physics for Geant4



https://doi.org/10.1016/j.nima.2023.168473

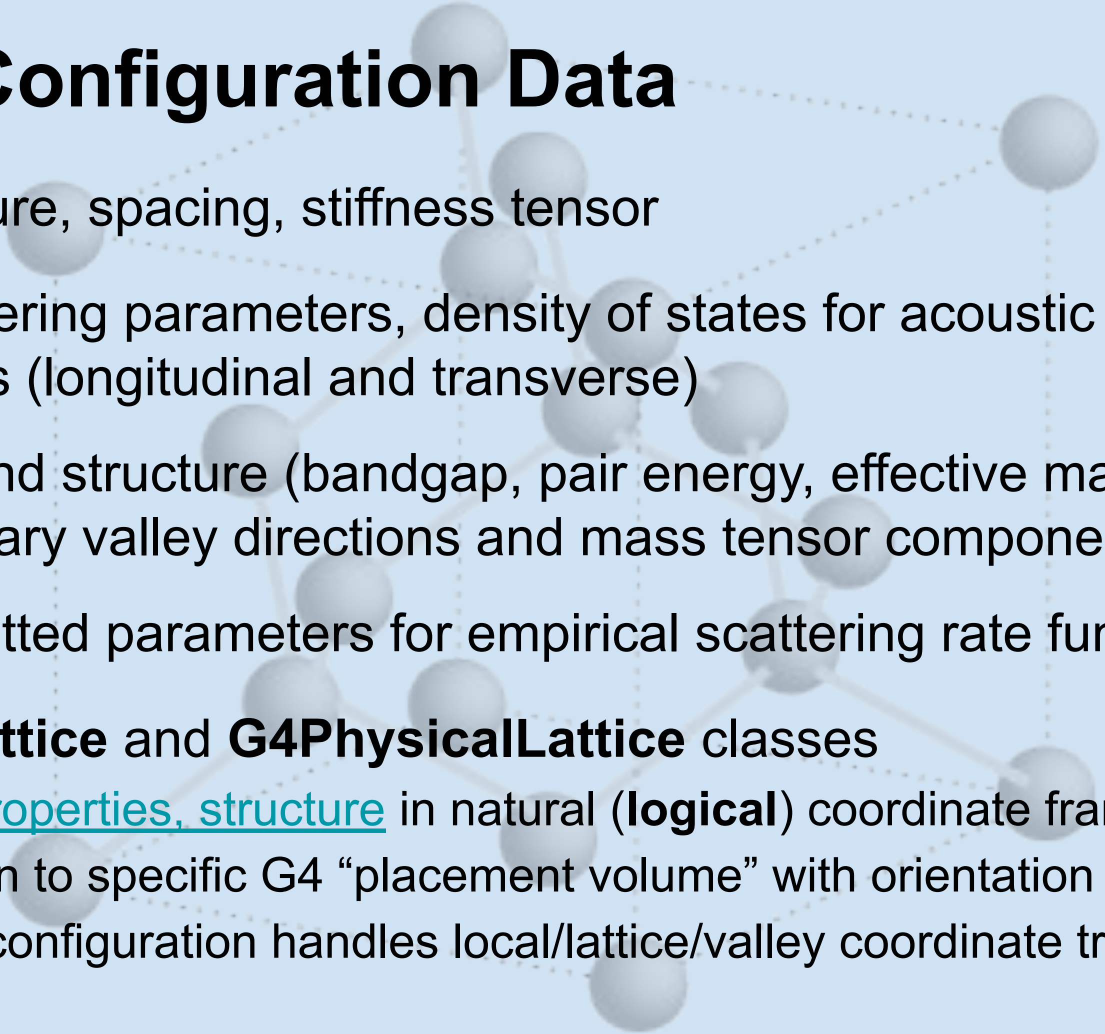
Atoms in a Crystal

Silicon and germanium both have diamond cubic lattice structure



	Ge	**Si**
Unit cell (a)	5.658 Å	5.431 Å
V_{sound} (L)	5.3 km/s	9.0 km/s
V_{sound} (T)	3.3 km/s	5.4 km/s
Band gap	0.74 eV	1.17 eV
Electron “effective mass”	1.59 m_e	0.95 m_e
Hole “effective mass”	0.35 m_e	0.50 m_e

Lattice Configuration Data



Lattice structure, spacing, stiffness tensor

Phonon scattering parameters, density of states for acoustic modes, sound speeds (longitudinal and transverse)

Electronic band structure (bandgap, pair energy, effective masses)
Electron primary valley directions and mass tensor components

Fano factor, fitted parameters for empirical scattering rate functions

G4LogicalLattice and **G4PhysicalLattice** classes

- Material properties, structure in natural (**logical**) coordinate frame of lattice
- Association to specific G4 “placement volume” with orientation (Miller indices)
- **Physical** configuration handles local/lattice/valley coordinate transforms

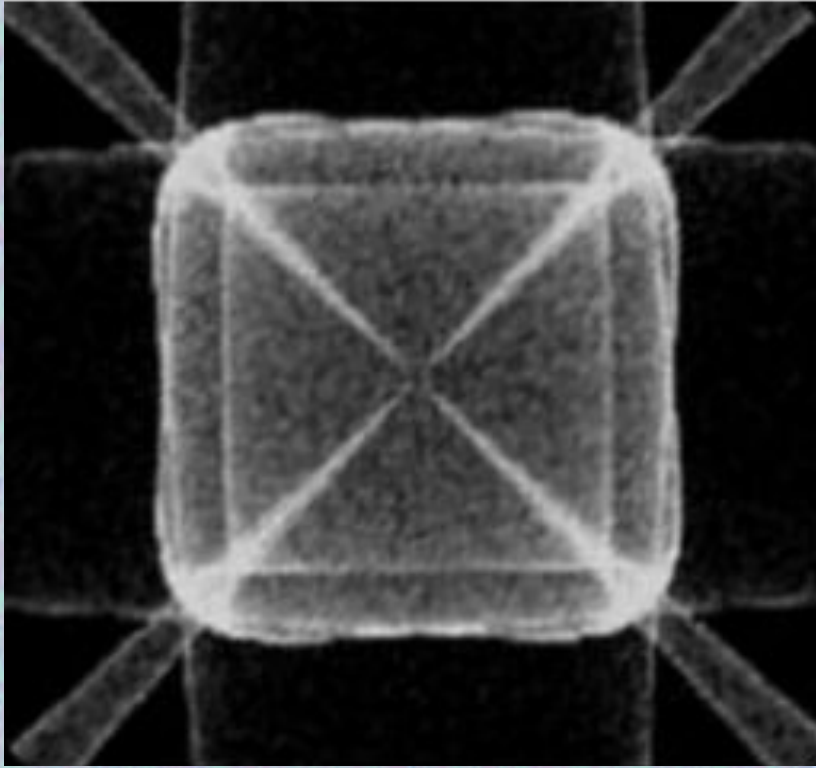
Phonon Transport

Quantized lattice oscillations

- Longitudinal (compression waves)
- Transverse (shear waves)

Lower energy (“acoustic”) and higher energy (“optical”) states

Dispersion relations, $\vec{v}_g = f(\vec{k})$, for each mode



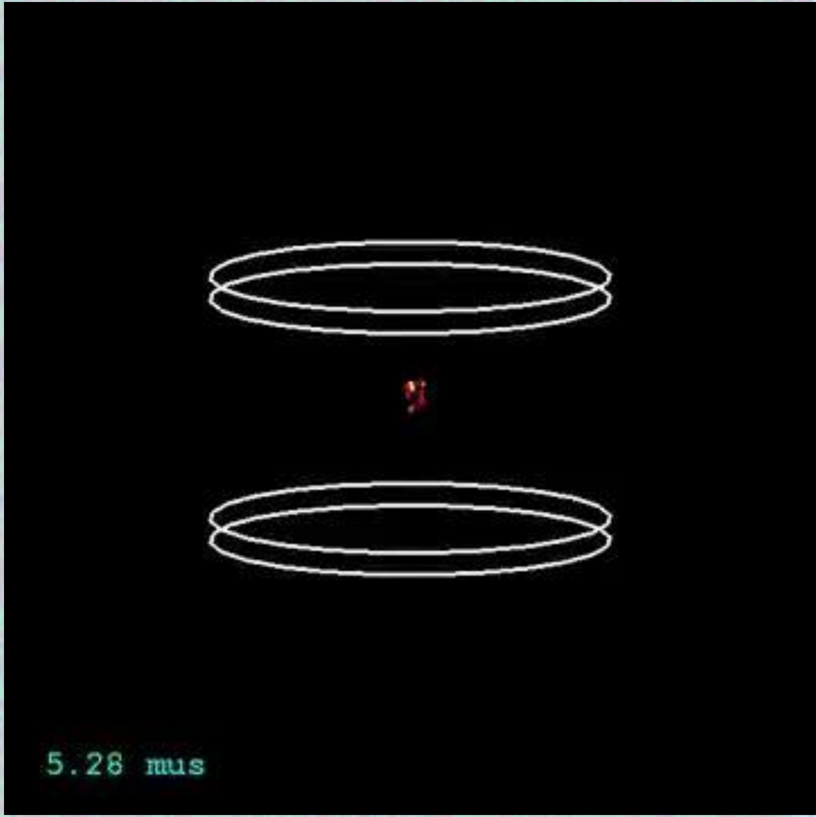
Phonon Scattering and Equipartition

Higher energy (tens of meV) phonons scatter off of impurities, different isotopes, crystal defects

Scatter and transform from one mode to another, rate ~ E^4

Some split into two lower energy phonons, rate ~ E^5

Low energy phonons rarely scatter



Charge Transport, Scattering and Valleys

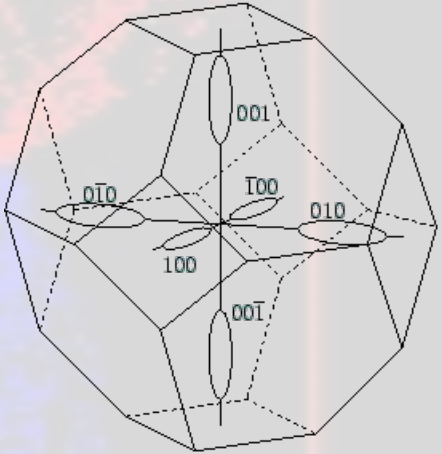
Incident particles promote electrons to conduction band, also creates holes (positive charge carriers)

Lowest energy bands have particular orientations (**valleys**)

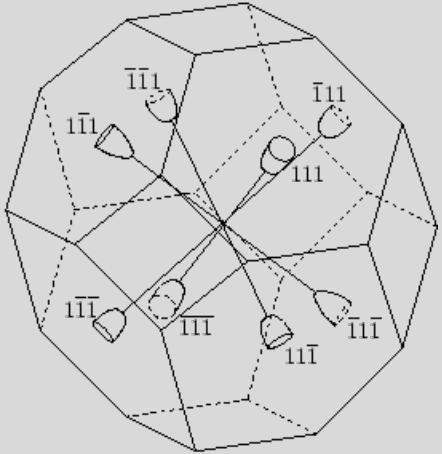
Electrons travel along valleys, with scattering between them

Charges accelerated in electric field radiate phonons

Charges interact with impurities, recombine with partner types



Silicon



Germanium

Neganov-Trofimov-Luke Phonon Emission

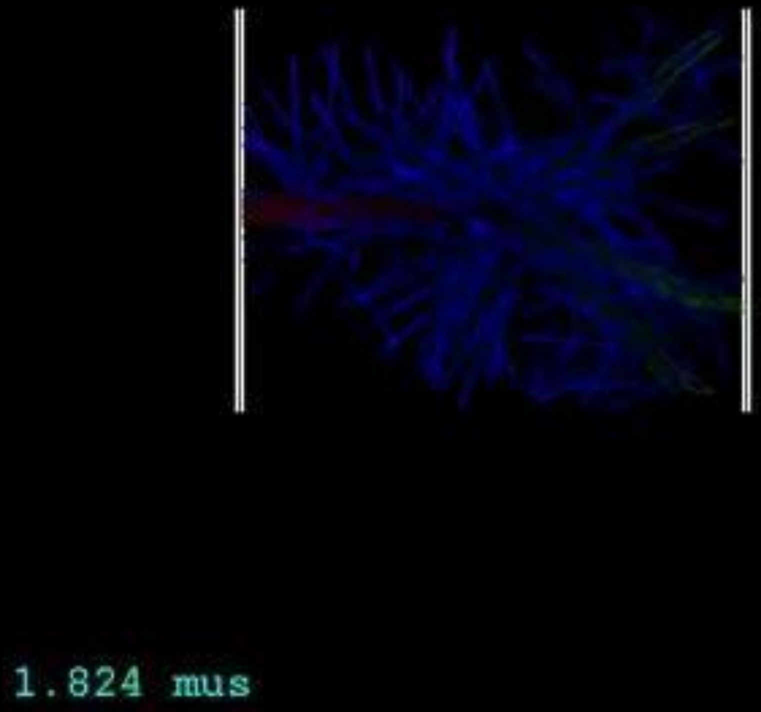
Charges accelerated in E-field pick up velocities well above v_{sound}

Interact with lattice to radiate phonons, reducing energy and changing direction

Rate $\nu = \frac{3\ell_0}{v_{\text{sound}}} \frac{Ma}{(Ma-1)^3}$

Total phonon emission equals energy gained from potential

G4CMPLukeScattering
G4CMPLukeEmissionRate



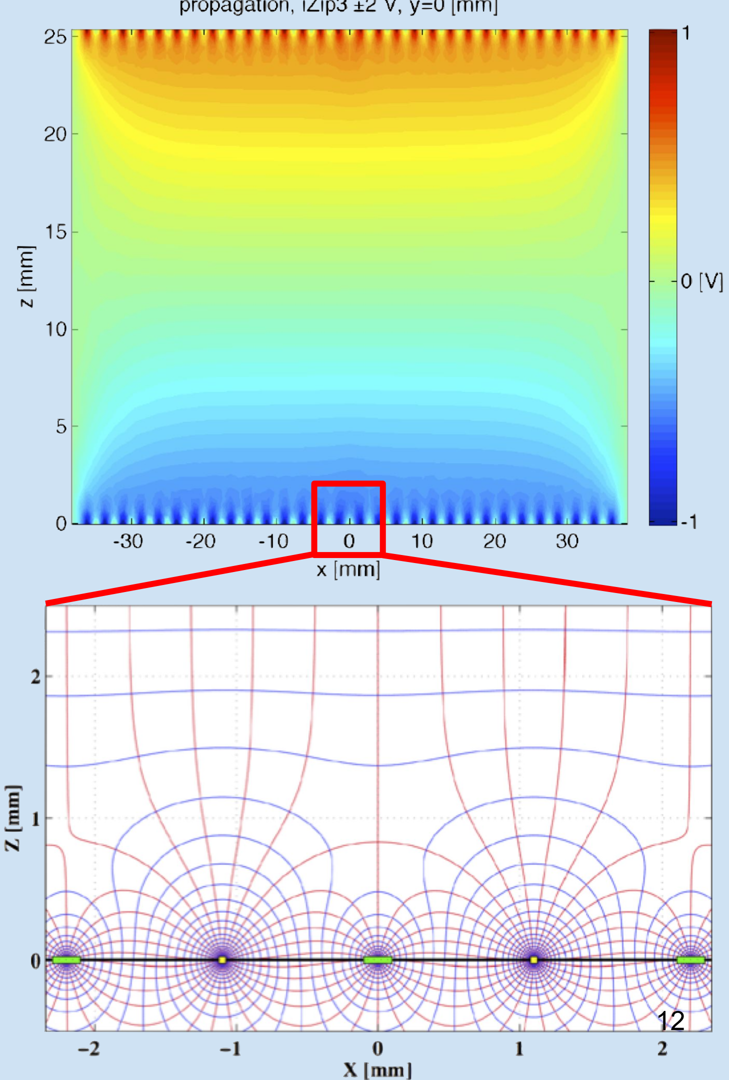
Finite Element Electric Field

Large detectors can have complex shapes and electrode layout

COMSOL, FEniCS, other physics modeling packages can generate a tetrahedral mesh of voltage at coordinates

G4CMPTriLinearInterp processes table of mesh points, tetrahedra

G4CMPLocalElectricField handles mesh in detector-local coordinates



Phonon Sensor Response

User-selectable class models phonon absorption on superconducting films, with energy collection and phonon emission

Thin-film superconductors in cryogenic sensors and QIS devices

- TES/QETs, KIDs, transmon qubits, ground planes

Model energy transfer, QP transport, phonon re-emission

- Phonon absorption can break pairs into electron quasiparticles
- Quasiparticles can lose excess energy by radiating phonons
- For small films, quasiparticle transport faster than thermal response

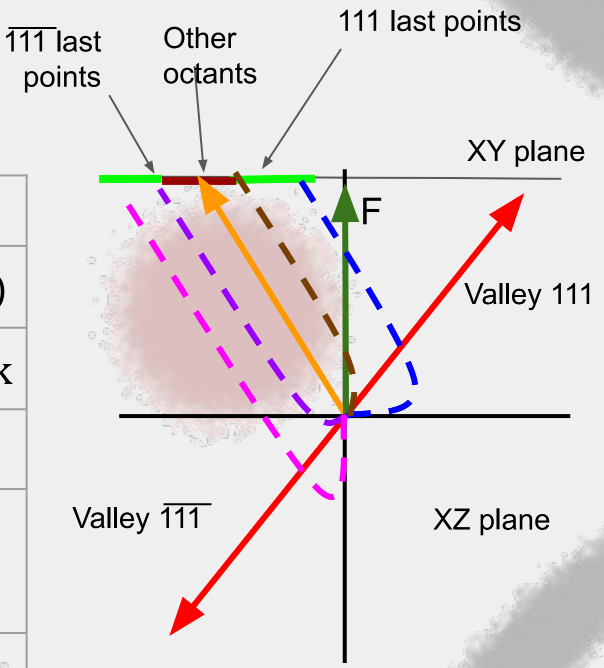
Film performance configurable with G4 material properties table

New Developments

Proper Electron Transport Kinematics

Wavevector momentum $p = \hbar k$ different from transport momentum $p =$ "mv", since "m" is tensor mass

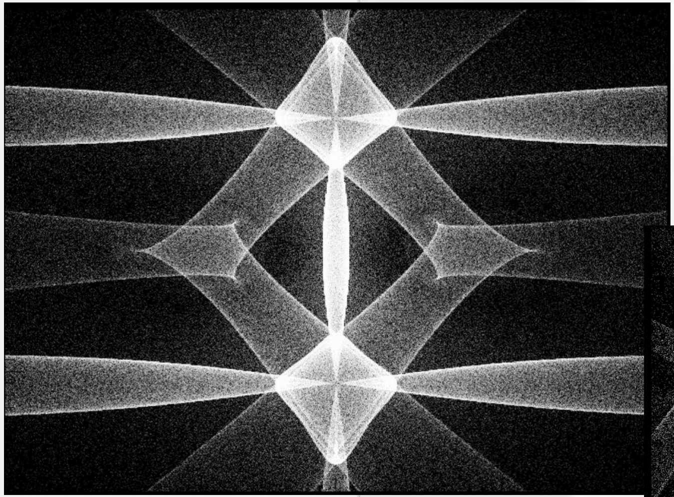
	Free Electron	**In Crystal**
Lorentz Boost	$\gamma^{-1} = \sqrt{(1-v^2/c^2)}$	$\gamma'^{-1} = \sqrt{(1-\mathbf{M}v^2/m_0c^2)}$
Transport Momentum	$P = \gamma\, m_0 v = \hbar k$	$P = \gamma'\, m_0 v = m_0 \mathbf{M}^{-1}\, \hbar k$
Kinetic Energy	$E_{kin} = (\gamma-1)\, m_0 c^2$	$E_{kin} = (\gamma'-1)\, m_0 c^2$
Effective Mass	$m(\vec{k}) = m_0$	$m(\vec{k}) = \dfrac{P^2c^2 - E^2_{kin}}{2\, E_{kin}\, c^2}$
Acceleration	$a = F/m_0$	$a = \mathbf{M}^{-1}\, F$



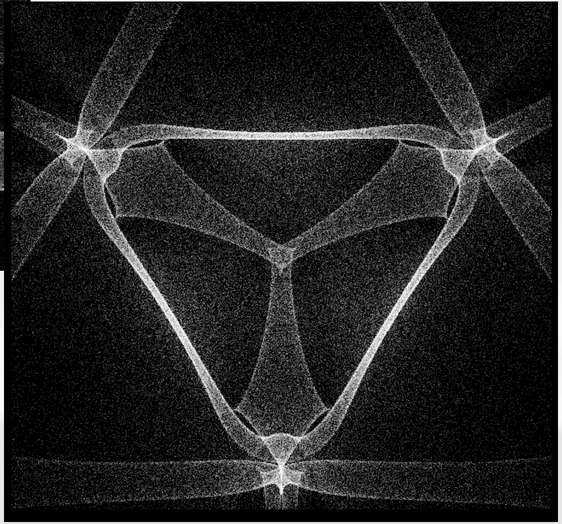
$\vec{a} = \mathbf{M}^{-1}\, \vec{F}$, not aligned!

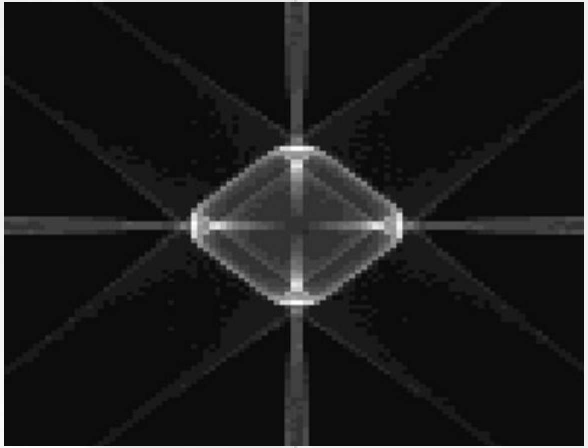
New Substrates: GaAs, Sapphire, LiF

Simulation: Caustics in 2 x 2 x 2 mm cubes


GaAs (110)

Sapphire (0001)

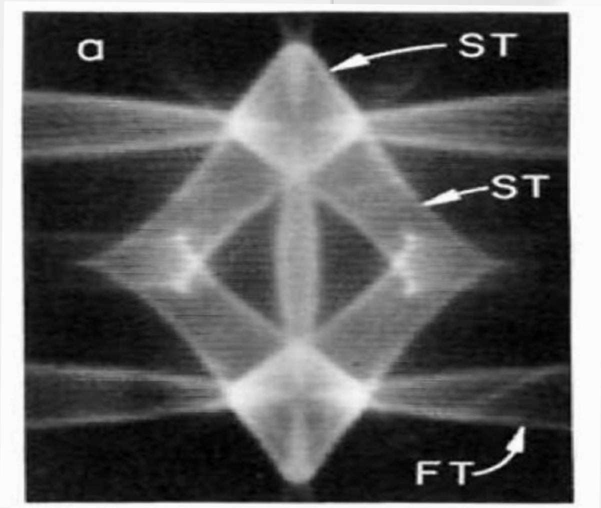



LiF (100)

I. Hernandez, IIT

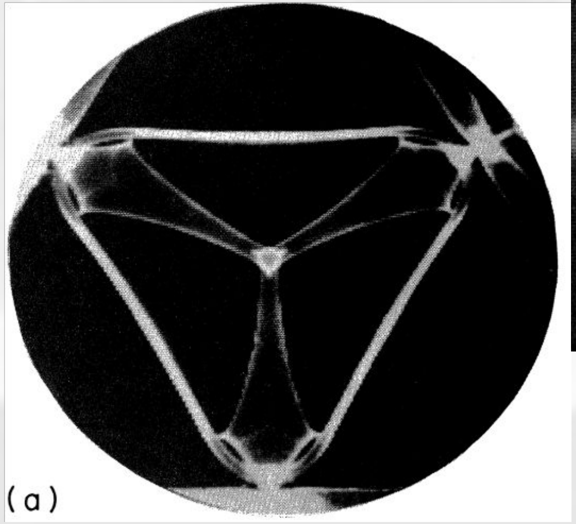
New Substrates: GaAs, Sapphire, LiF

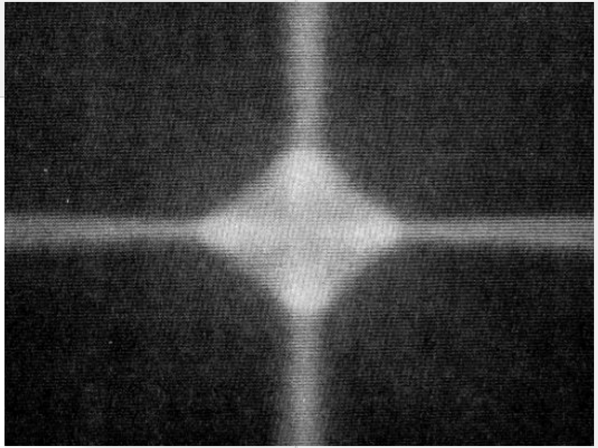
Experimental Measurements



GaAs (110)

Sapphire (0001)





LiF (100)

I. Hernandez, IIT

Quasiparticle Transport in Thin Films

Support for tracking both phonons and Bogoliubov QPs in superconducting films layered on a substrate

- Incident phonons create "hot" QP pairs in film
- Phonon scattering on grain boundaries
- Phonon "escape" from film back into substrate
- QP radiation of phonons down to energy gap Δ
- QP recombination in film and emission of 2Δ phonon(s)
- QP diffusion (not single-scatter tracking)

Software Info and Discussion

A Side Note About Geant4 Limitations

Geant4 was designed primarily for the high energy physics community, and its overall structure reflects that:

- Individual particles propagate one at a time through a static universe of materials and fields
- Every event starts over in the same universe, at time $t=0$
- Particles do not alter the features of the universe: no charge buildup, no material activation or structural degradation, no "population density," etc.
- Particles do not interact with one another
- Each particle propagates forward in time, but the order in which particles are processed in an event does not have any time order

Where to Get G4CMP?

https://github.com/kelseymh/G4CMP.git

README file describes how to build, configuration parameters

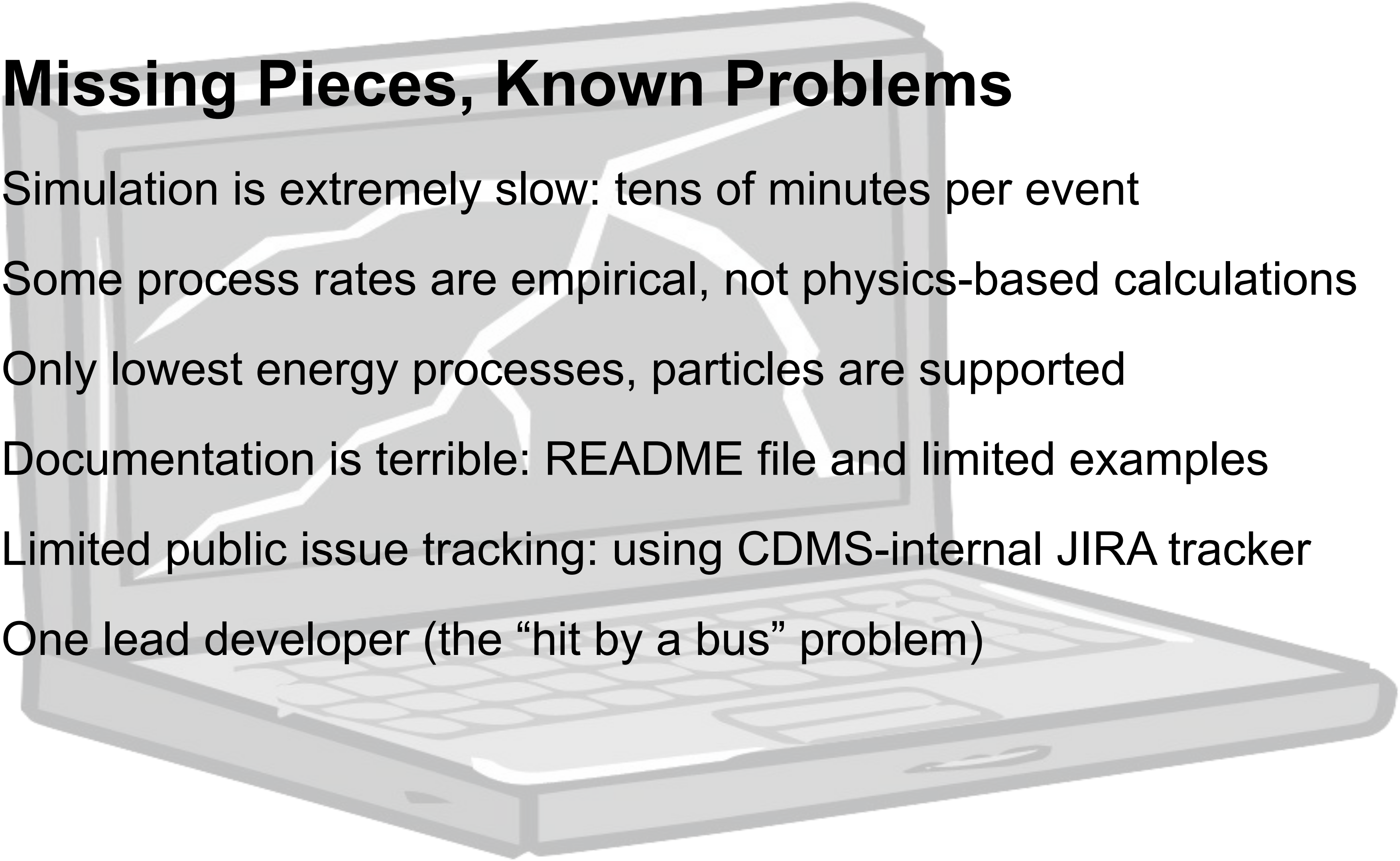
Example standalone applications in distribution (very limited)

Publication: NIM A 1055 (2023) 168473 (arXiv:2302.05998)

Builds with CMake or GNU Make

- Must have Geant4 installed, envvars set
- Physics list for standalone “G4CMP-only” simulations
- Physics builder for integration with Geant4 simulations

Missing Pieces, Known Problems



Simulation is extremely slow: tens of minutes per event

Some process rates are empirical, not physics-based calculations

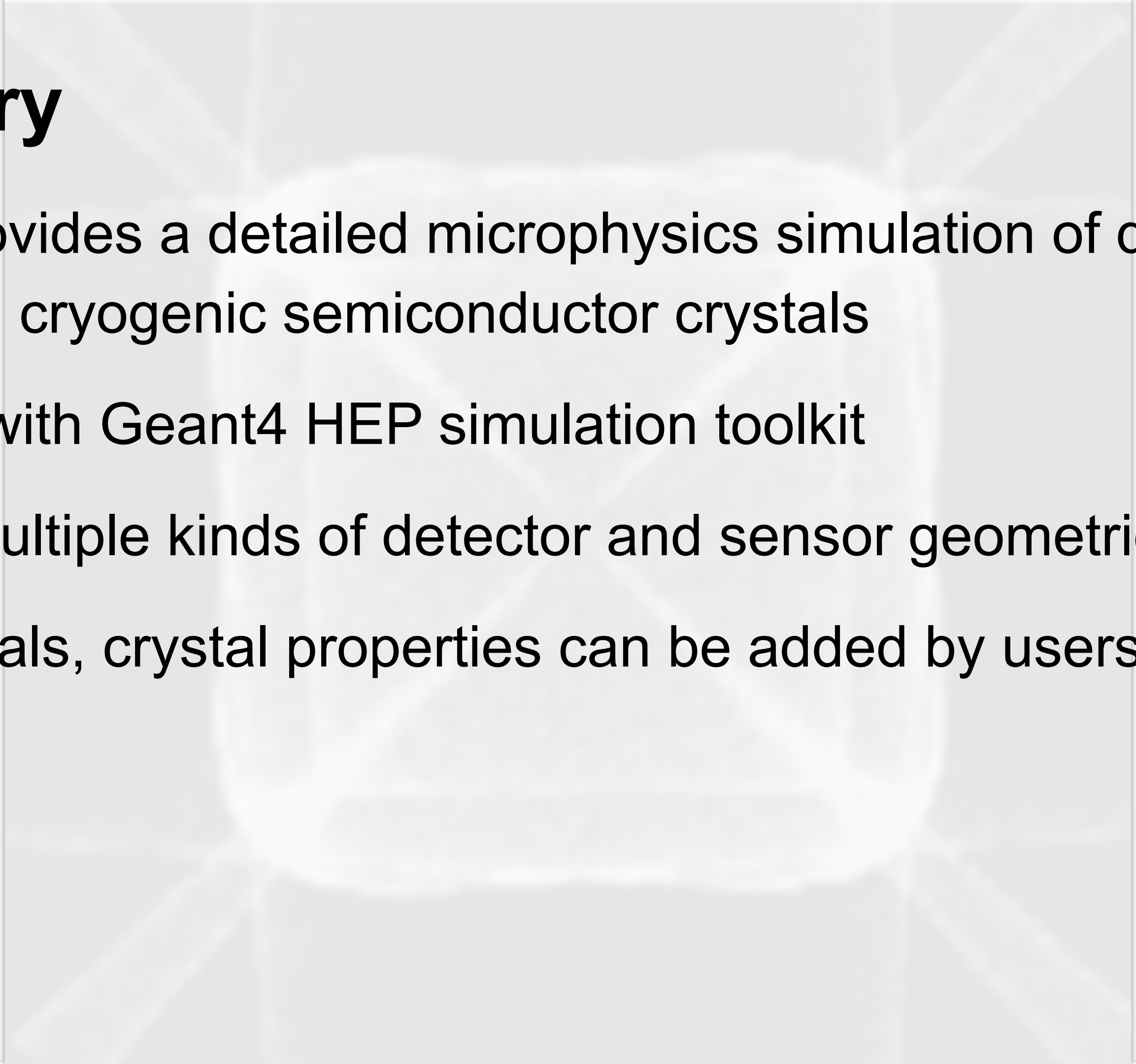
Only lowest energy processes, particles are supported

Documentation is terrible: README file and limited examples

Limited public issue tracking: using CDMS-internal JIRA tracker

One lead developer (the “hit by a bus” problem)

Summary



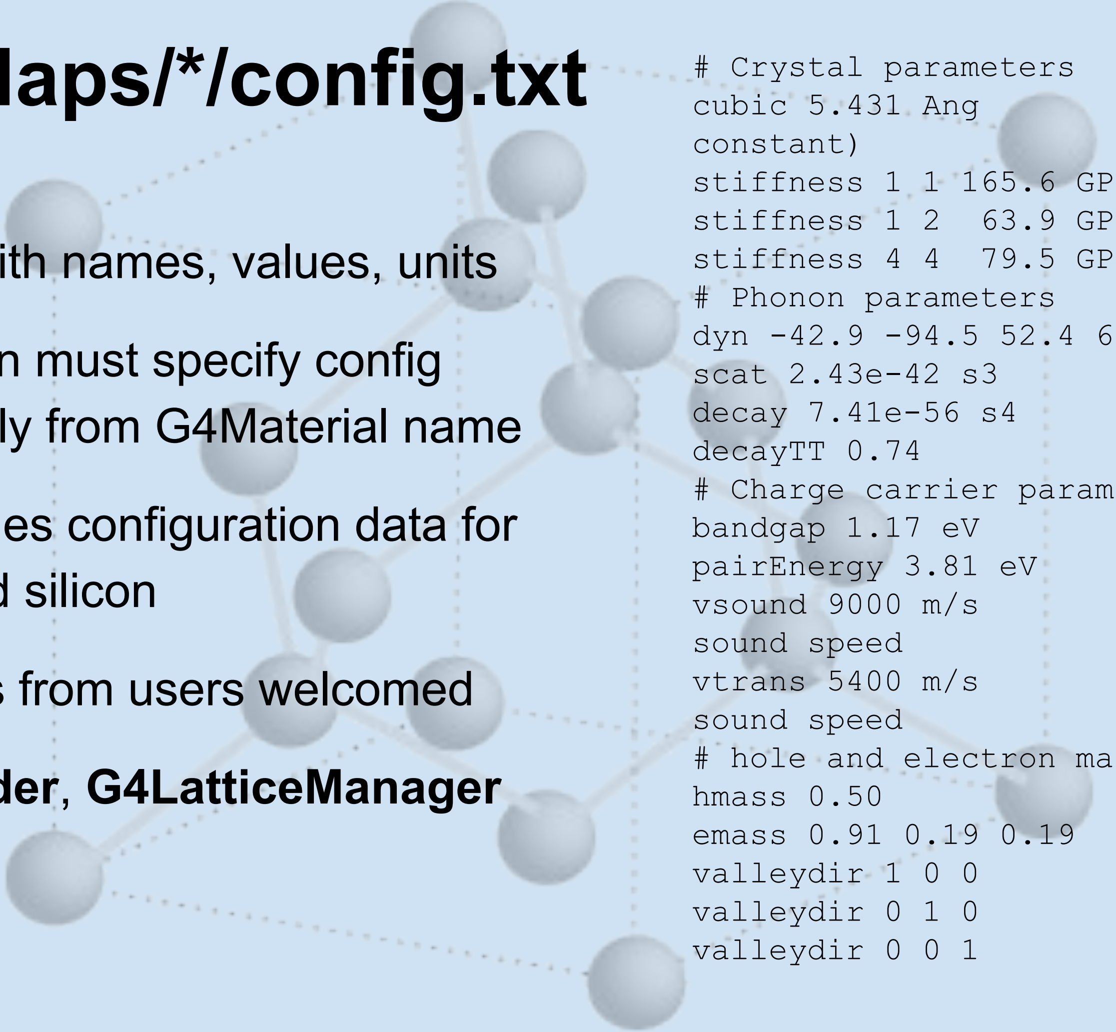
G4CMP provides a detailed microphysics simulation of detector response in cryogenic semiconductor crystals

Integrated with Geant4 HEP simulation toolkit

Supports multiple kinds of detector and sensor geometries

New materials, crystal properties can be added by users

Backup Slides and Details



CrystalMaps/*/config.txt

Plain text file with names, values, units

User application must specify config name separately from G4Material name

Package includes configuration data for germanium and silicon

Other materials from users welcomed

G4LatticeReader, **G4LatticeManager**

```
# Crystal parameters
cubic 5.431 Ang         # (Lattice
constant)
stiffness 1 1 165.6 GPa # C11, C12, C44
stiffness 1 2  63.9 GPa
stiffness 4 4  79.5 GPa
# Phonon parameters
dyn -42.9 -94.5 52.4 68.0 GPa
scat 2.43e-42 s3
decay 7.41e-56 s4
decayTT 0.74
# Charge carrier parameters
bandgap 1.17 eV
pairEnergy 3.81 eV
vsound 9000 m/s         # Longitudinal
sound speed
vtrans 5400 m/s         # Transverse
sound speed
# hole and electron masses
hmass 0.50              # per m(electron)
emass 0.91 0.19 0.19    # per m(electron)
valleydir 1 0 0
valleydir 0 1 0
valleydir 0 0 1
```

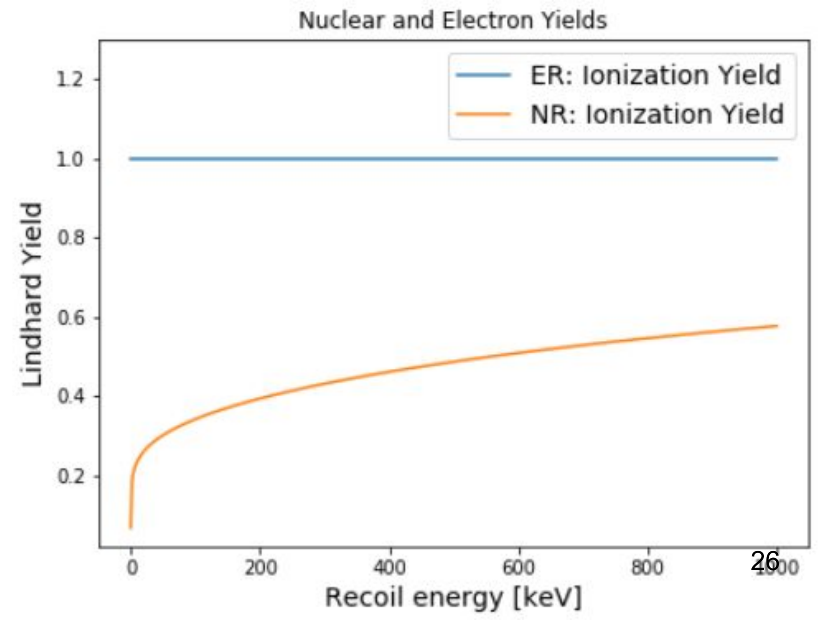
Lindhard/Robinson or Lewin/Smith Partition

Relative magnitude of dE/dx vs. NIEL for ions depends on charge and mass of projectile, and atomic number and mass of crystal atoms

Compute "Yield": dE/dx fraction of total

- Done in G4CMP code for ion hits
- Now done automatically in Geant4 10.7
- Forward compatible (if non-zero NIEL, G4CMP will not recalculate)

G4CMPLindhardNIEL
G4CMPLewinSmithNIEL



Phonon Transport Processes

Phonon Mode Group Velocity

Use crystal stiffness matrix along a given direction $\hat{\mathbf{n}}$

- Christoffel matrix $D_{il} = C_{ijlm} \cdot \hat{n}^{j} \cdot \hat{n}^{m} / \rho$
- Eigenmodes are phase velocity and polarization

From those, group velocity is computed

For speed in processing, lookup tables are generated

- Steps of $\hat{\mathbf{n}}$ coordinates
- Interpolated between steps

G4CMPPhononKinematics

Phonon Impurity Scattering

Phonon scattering off of impurities can change their mode, from longitudinal (L) to slow (ST) or fast transverse (FT), etc.

Rate scales like E^4, with scattering constant: $\nu = \mathrm{B}\cdot(\mathrm{E}/h)^4$

- $\mathrm{B} = 2.43\times10^{-42}\ \mathrm{s}^3$ (Si)

Implemented with wavevector (energy) conservation

- Choose different mode based on configured density of states
- Use wavevector to determine new velocity vector

G4PhononScattering, **G4CMPPhononScatteringRate**

Phonon Anharmonic Decays

Longitudinal (L) phonons scatter and “decay” into pairs

- L → T T or L → L’ T

Rate scales like E^5, with decay constant: $\nu = \mathrm{D}\cdot(\mathrm{E}/h)^5$

- $\mathrm{D} = 2.43\times10^{-42}\ \mathrm{s}^3$ (Si), TT / L’T fraction 74% (Si)

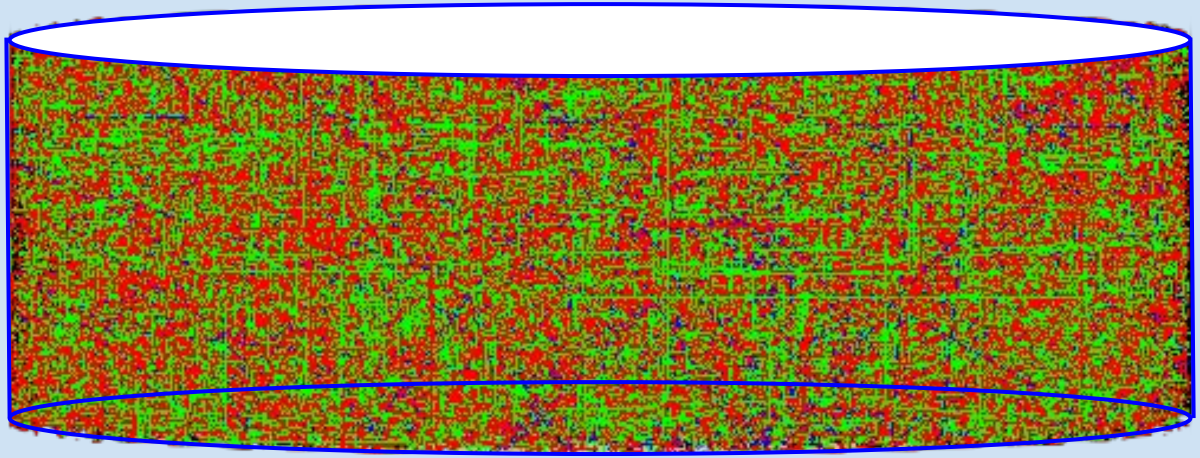
Equipartitions early “hot” (Debye energy, tens of meV) phonons into sea of meV-scale phonons

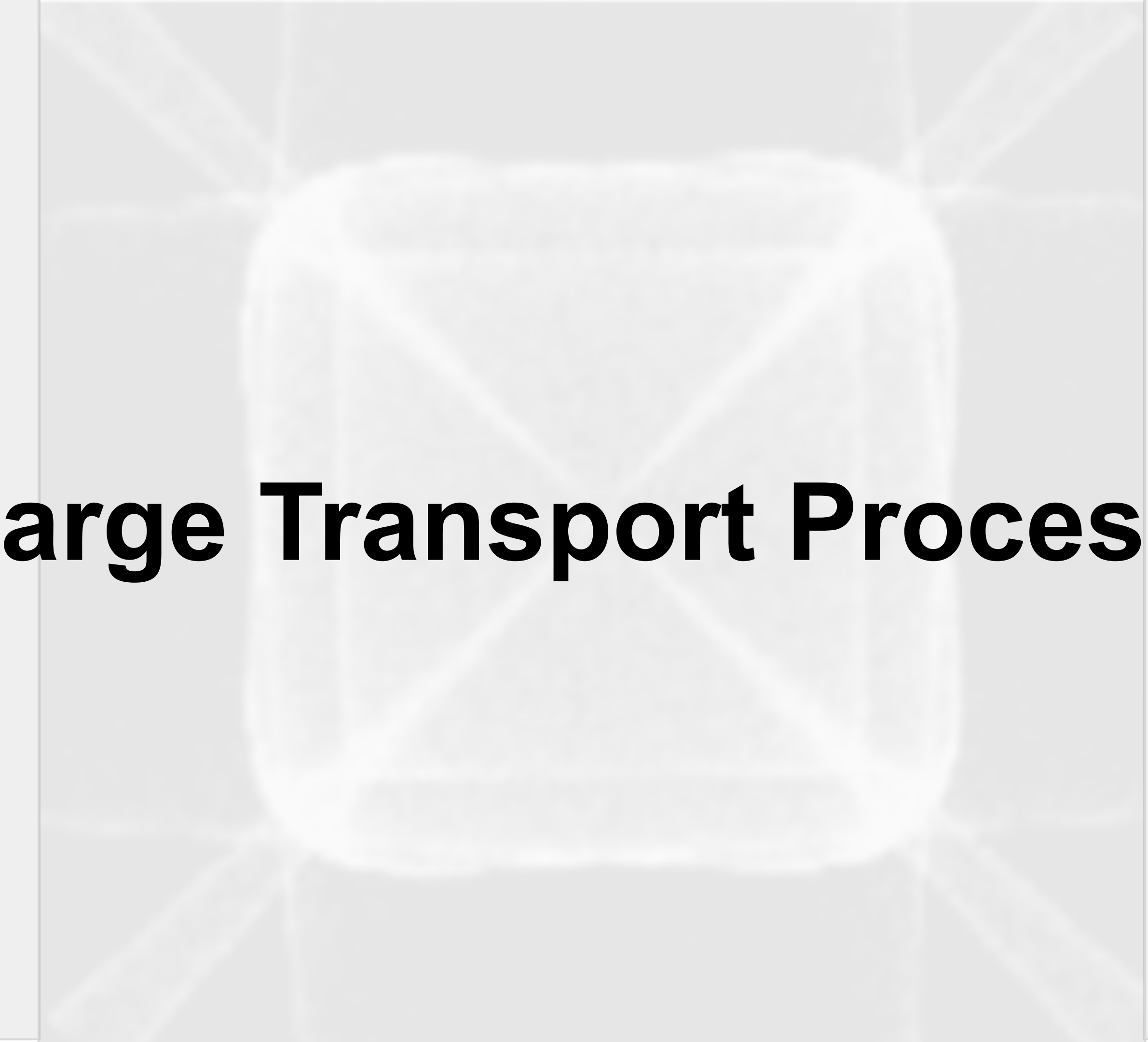
G4PhononDownConversion, **G4CMPDownconversionRate**

Phonons: Scattering and Equipartition

After energy deposit, crystal filled with “gas” of low energy ($\lesssim$ meV) phonons, with all modes represented, moving in all directions

Sensors on top and bottom can absorb phonons to measure energy





Charge Transport Processes

Electron Mass Tensor

Electron transport along a valley

- Different effective masses parallel vs. perpendicular to valley axis
- Could have different masses in multiple directions

Let valley axis be $\vec{x}$, $\mathbf{M} = \begin{bmatrix} m_\perp & 0 & 0 \\ 0 & m_\perp & 0 \\ 0 & 0 & m_\parallel \end{bmatrix}, \vec{p} = \mathbf{M}\vec{v}, E = \vec{p}^T\mathbf{M}\vec{p}$

Relationship only applies close to valley axis

- Mass tensor is direction dependent in general
- G4CMP uses fixed mass tensor for all kinematics

Electron Intervalley Scattering

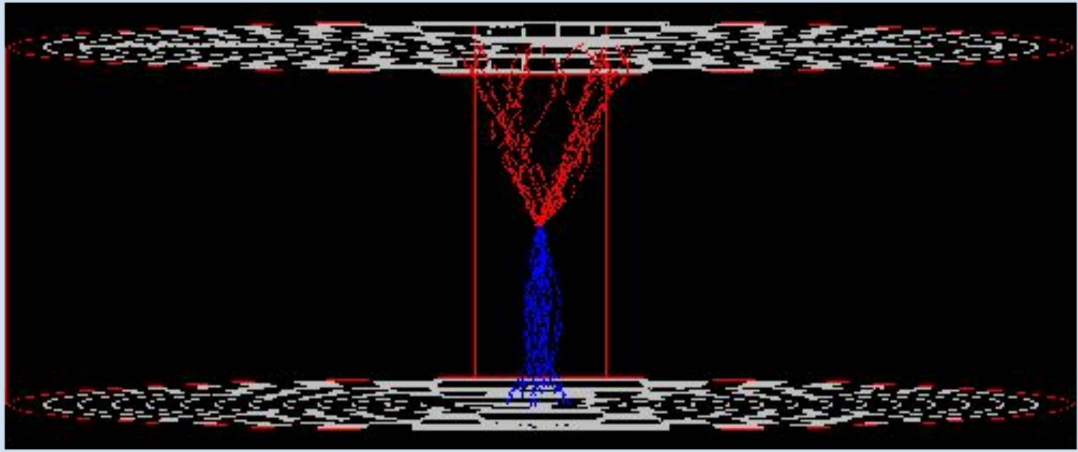
Electrons may be strongly scattered by absorption of thermal phonons

Large momentum transfer to move electron from one valley to another

IV scattering contributes to electron drift speed; fit rate to E field

G4CMPInterValleyScattering

- **G4CMPIVRateLinear**
- **G4CMPIVRateQuadratic**
- **G4CMPInterValleyRate**



Charge Recombination

Particles in G4 independent and isolated (don’t mutually interact)

Charges (e, h) at surfaces cannot escape, do not “reflect” vs. bias

Assume they recombine with some pre-existing partner (e+h, h+e)

Half of bandgap energy released as phonons at Debye frequency

- 15 THz, 62.03 meV (Si); 2 THz, 8.27 meV (Ge)
- If e/h pairs were created initially, *half* from each ensures energy conservation

G4CMPDriftRecombinationProcess

Charge Trapping on Impurities

Similar to recombination: charges stopped by impurities in bulk

Shallow (~ meV) depth, bandgap energy not recovered

Two impurities: four kinds of capture, with separate rates for e, h

- $e + D^0 \rightarrow D^-$, $e + A^+ \rightarrow A^0$, $h + A^0 \rightarrow A^+$, $h + D^- \rightarrow D^0$

Stopped charges can contribute to charge collection signal, if near electrodes

G4CMPDriftTrappingProcess

```
/g4cmp/electronTrappingLength
/g4cmp/holeTrappingLength
```

Rates can be device dependent, and even history (neutralization) dependent

Impurity Trap Reionization

Inverse to trapping: tracks can interact with traps, releasing charges

Shallow (~ meV) depth, bandgap energy not absorbed

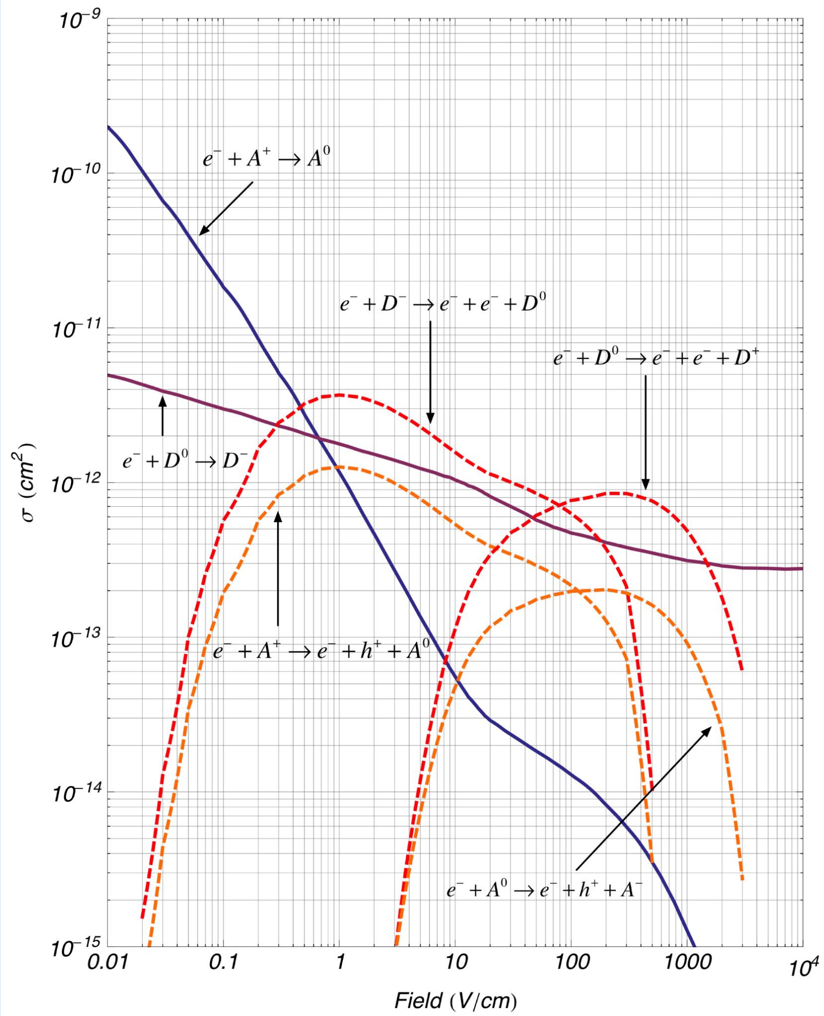
Two impurities, four kinds of reionization, with separate rates

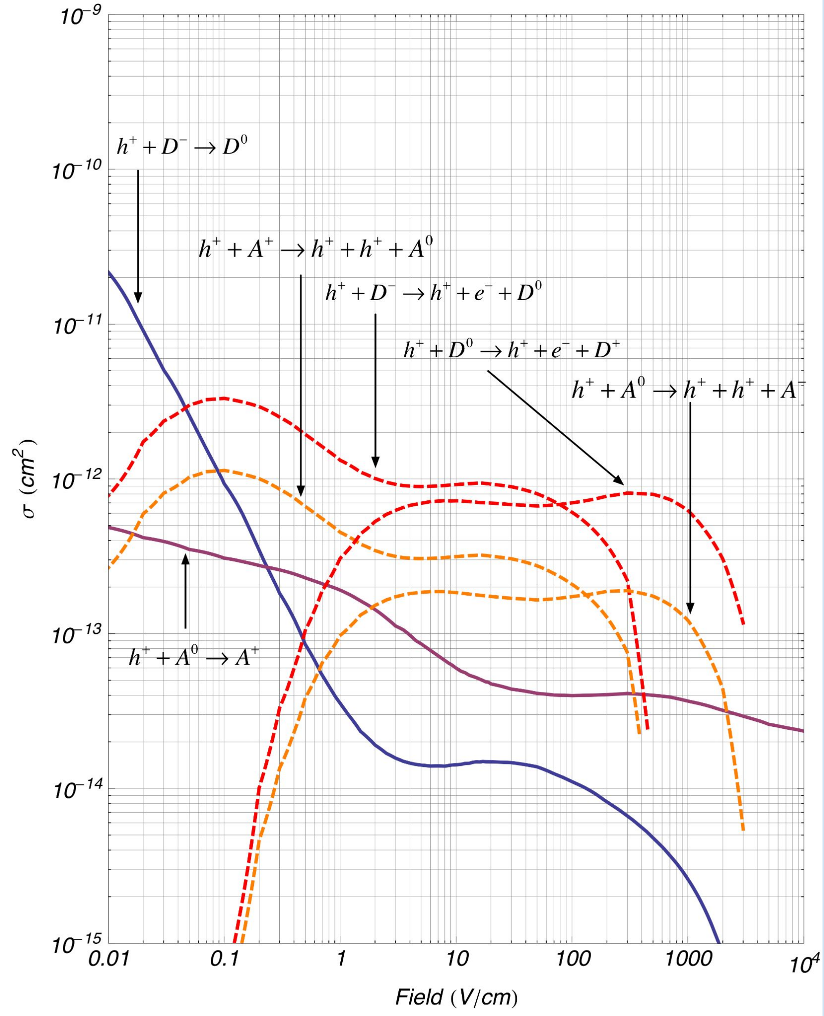
- $e + D^{-} \rightarrow 2\,e + D^{0}$, $e + A^{+} \rightarrow e + h + A^{0}$
- $h + A^{0} \rightarrow 2\,h + A^{+}$, $h + D^{-} \rightarrow h + e + D^{0}$

G4CMPDriftTrapIonization

```
/g4cmp/eDTrapIonizationMFP
/g4cmp/eATrapIonizationMFP
/g4cmp/hDTrapIonizationMFP
/g4cmp/hATrapIonizationMFP
```

Rates can be device dependent, and even history (neutralization) dependent


10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
$\sigma\ (cm^2)$
0.01
0.1
1
10
100
1000
10^4
Field (V/cm)
$e^- + A^+ \rightarrow A^0$
$e^- + D^- \rightarrow e^- + e^- + D^0$
$e^- + D^0 \rightarrow e^- + e^- + D^+$
$e^- + D^0 \rightarrow D^-$
$e^- + A^+ \rightarrow e^- + h^+ + A^0$
$e^- + A^0 \rightarrow e^- + h^+ + A^-$


10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
$\sigma\ (cm^2)$
0.01
0.1
1
10
100
1000
10^4
Field (V/cm)
$h^+ + D^- \rightarrow D^0$
$h^+ + A^+ \rightarrow h^+ + h^+ + A^0$
$h^+ + D^- \rightarrow h^+ + e^- + D^0$
$h^+ + D^0 \rightarrow h^+ + e^- + D^+$
$h^+ + A^0 \rightarrow h^+ + h^+ + A^-$
$h^+ + A^0 \rightarrow A^+$

Energy Partitioning in G4CMP

Geant4 typically doesn’t produce “trackable” electrons below tens of eV, just records “energy deposit” value associated with parent track

- dE/dx summarizes all the conduction electrons produced by track
- Minimum energy required for one e/h pair is **bandgap**, ~1 eV
- Typically, **pair energy** (~3-4 eV) per e/h pair, with variation

Ions (including alphas) induce motion of nearby atoms in lattice

- Non-ionizing energy loss (NIEL)
- Athermal phonons, each with Debye energy (tens of meV)

G4CMPSecondaryProduction, **G4CMPEnergyPartition**

Superconducting Films

G4CMPKaplanQP

Simulation treated as instantaneous

- Iterates to find equilibrium state, no time-dependent info

Substrate phonon absorbed on film

- Use mean free path (from lifetime $\boldsymbol{\tau}$) and thickness *d* for probability
- $\mathrm{P} = \exp(-4d/\mathrm{MFP})$ $\mathrm{MFP} = \mathrm{v}_{\mathrm{sound}}/\boldsymbol{\tau}(\mathrm{E})$ $\boldsymbol{\tau}(\mathrm{E}) = \boldsymbol{\tau}_0 \,/\, (1 + \delta\boldsymbol{\tau}\cdot(\mathrm{E}/\boldsymbol{\Delta} - 2))$

Phonon energy goes to break Cooper pairs (“QP energy”)

QP or phonon energy absorbed onto tungsten TES

- Some QP energy goes back into phonons via QP “decay” (emission)
- Some phonon energy re-emitted back into substrate

Processing loop ends when available phonon energy is zero

- Not suitable for “bare” films without attached energy sink

Quasiparticle Transport in Thin Films

Phonon scattering on grain boundaries

- Use MFP or "effective rate"; single-scatter explodes CPU time

Phonon-induced QP cascades

- Processes equivalent to what "0D" KaplanQP currently does
- QP energy loss by emission of phonons, creation of QP pairs from phonons
- Phonon "escape" from film back into substrate

QP recombination in film and emission of 2Δ phonon(s)

- Assumes recombination with existing QP bath is dominant
- NO recombination between multiple generated QPs

QP diffusion with effective methods challenging: multiple length scales

Phonon Readout Model (SuperCDMS)

Phonon energy deposit collected in time bins, matching readout

Coupled differential equations model electrothermal response of TESes, bias current, inductive (SQUID) coupling, etc.

Use CVODE (from LLNL) to solve for current output in each time bin

Configuration files specify detector components, characteristics

- Heat flow, resistances, inductance, TESes per channel, etc.

Some Applications of G4CMP

SuperCDMS Detectors

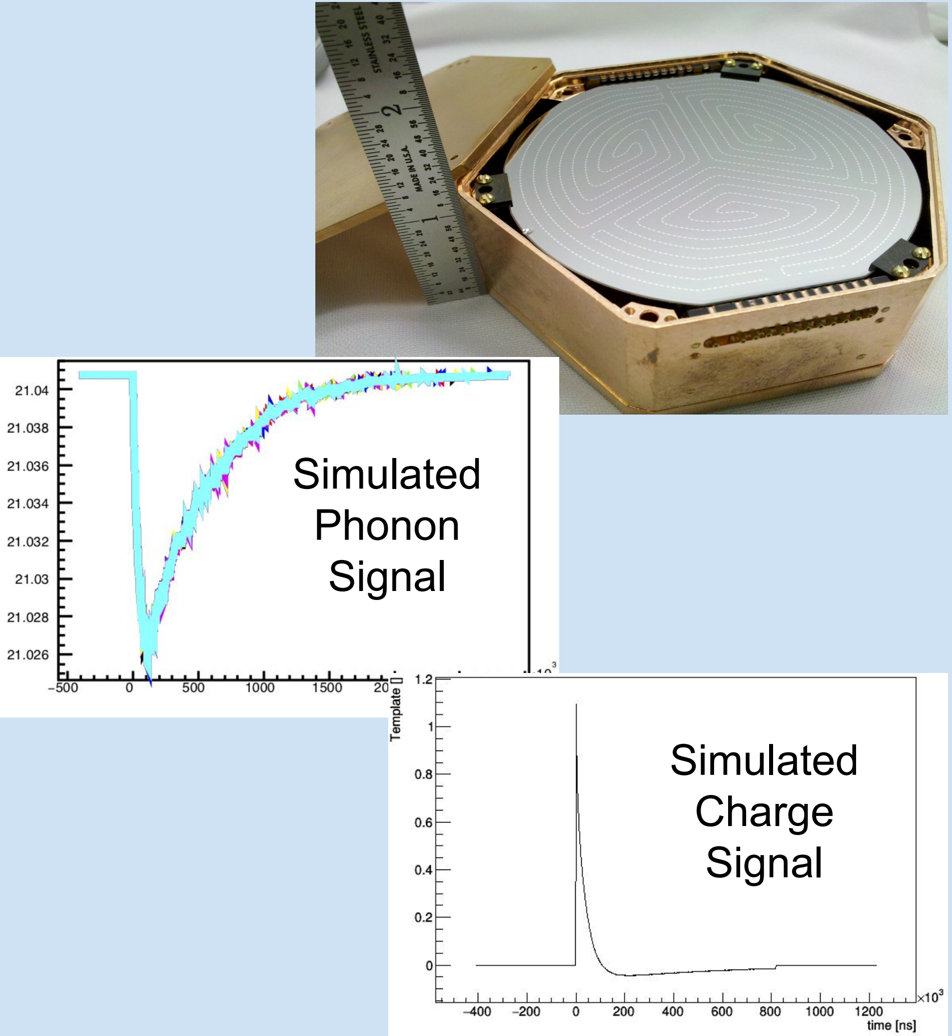
100 mm D x 33 mm Ge(100) or Si(100) crystal

9,540 TESes with phonon-collection fins on each side, connected in parallel (six channels), with voltage bias lines interleaved

400 ns readout digitization gives time resolved signals, showing the phonon population in the detector decaying away after an energy deposit

Charge collection "decay" and "recovery" are determined by the capacitance of the detector and the readout reistances

Time dependent readout signals modeled with [equations for circuit response]()



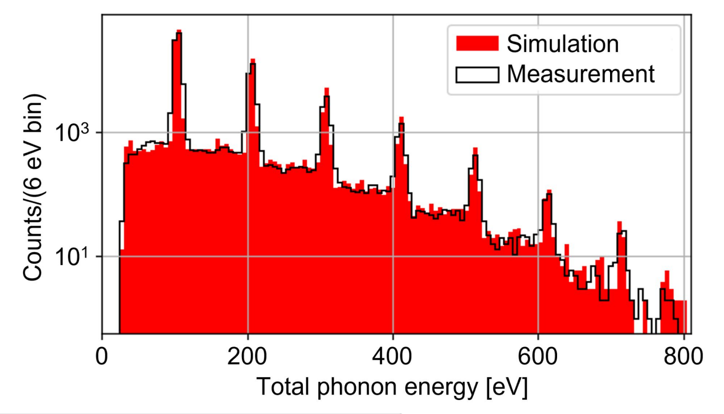
HVeV Detector QETs with Readout

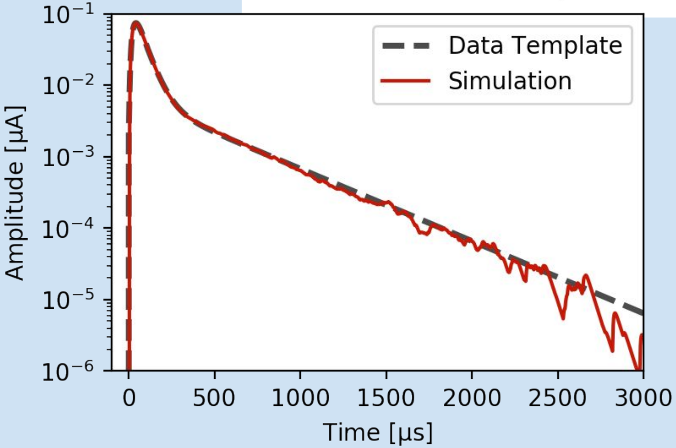
R&D for ultra-low threshold (single e/h resolution) dark matter detectors

10 x 10 x 4 mm chip, 20% coverage with phonon sensors (QETs)

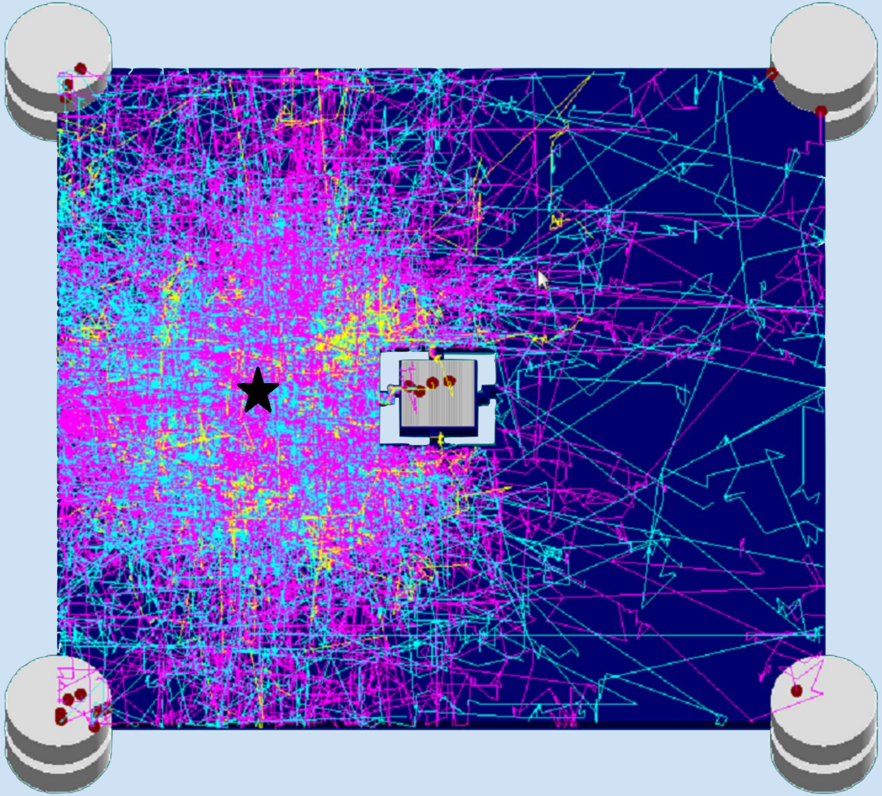
G4CMP reproduces single e/h peaks, energy scale, and "background" due to charge trapping and trap ionization

G4CMP + ODE reproduces shape of readout signal over four orders of magnitude





Phonon-Isolated Superconducting Sensor



2 x 2 mm superconducting device, isolated from silicon support structure with trenching and small "legs"

Phonons generated istropically at indicated position ★ in substrate

Red points indicate phonon absorption in device or at corner clamps

Phonon transfer into device is minimal, scales with width of legs

Other Groups Using G4CMP

LiteBIRD : CMB experiment, superconducting polarimeters

Spatial Imaging of Charge Transport in Silicon (C.Stanford *et al.*)

Athermal Phonons in KID Sensors (M.Martinez *et al.*)

Superconducting Qubits (Several groups at FNAL, PNNL, others)

Low-mass, High-sensitivity Particle Detectors (CDMS R&D groups)