SuperCDMS: Detector Simulation with G4CMP

Michael H. Kelsey, Texas A&M

HEP Software Foundation

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Overview

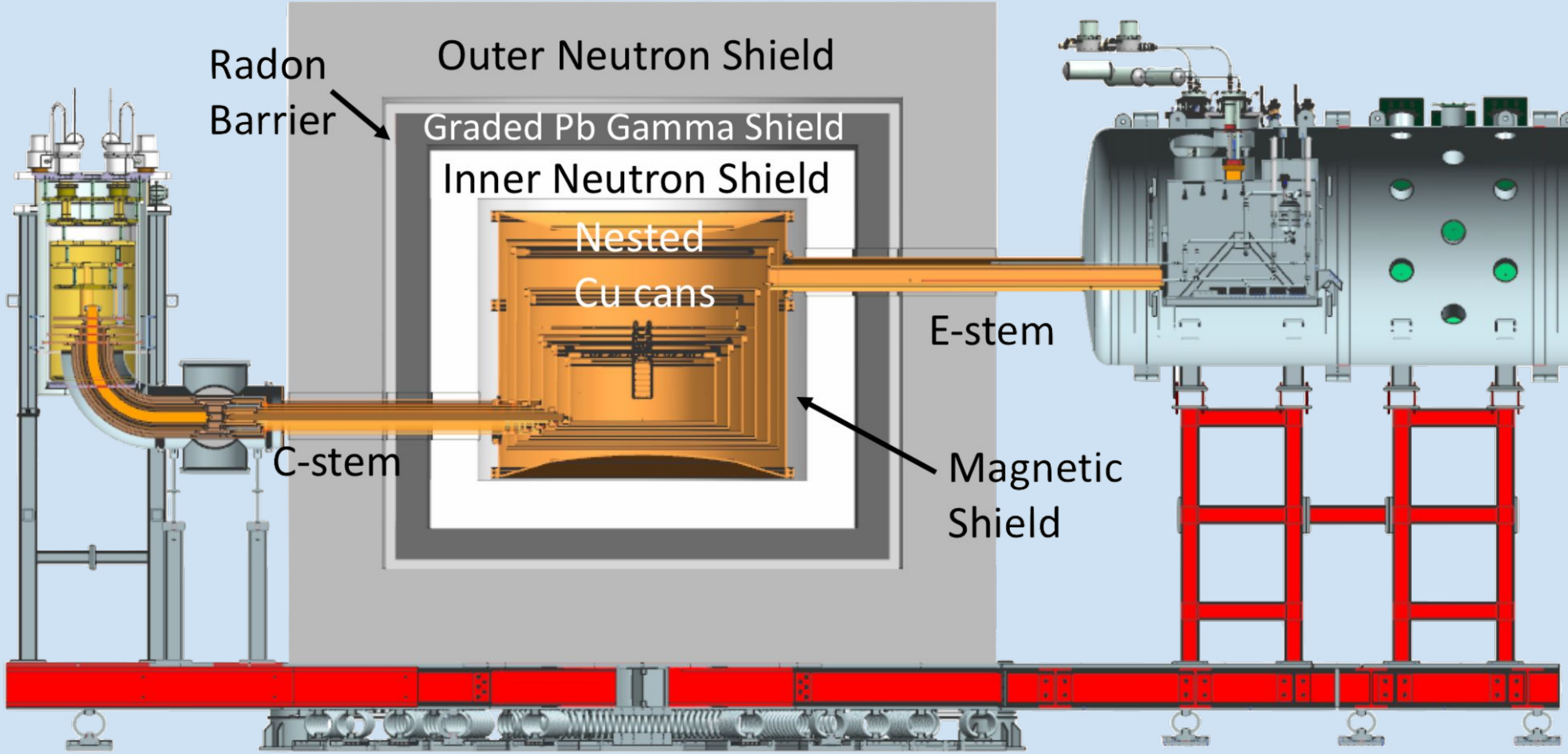
SuperCDMS is a dark matter search using cryogenic semiconductor crystals. We are using Geant4 and the G4CMP package to simulate the detector response to backgrounds and dark matter.

- SuperCDMS Experiment
- Simulations and the G4CMP Package
- Bits of Solid State Physics
- Sensor Simulation, Modeling
- Software Info and Discussion

Hyperlinks connect to appropriate backup slides

SuperCDMS Detectors

SuperCDMS Experiment



Detector Towers

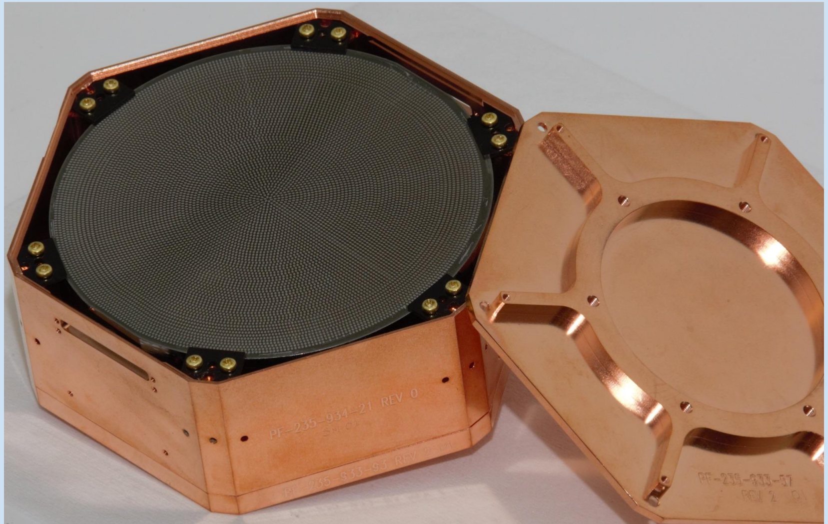
50 mK base temperature, 6-stage fridge

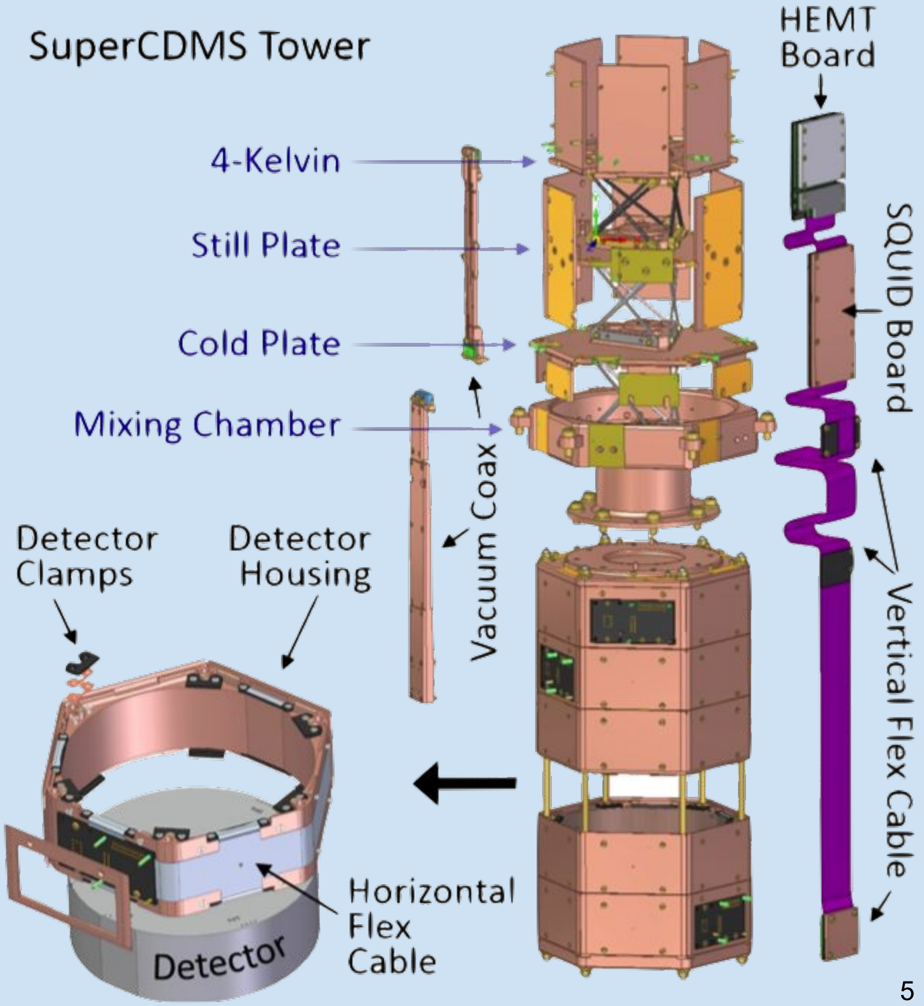
4 towers, 6 detectors each

Germanium, silicon detectors

High (100V) and low (4V) voltage

Charge and phonon sensors





SuperCDMS Detectors

High purity single crystals, 100×33 mm thick, 0.6 (Si), 1.5 (Ge) kg

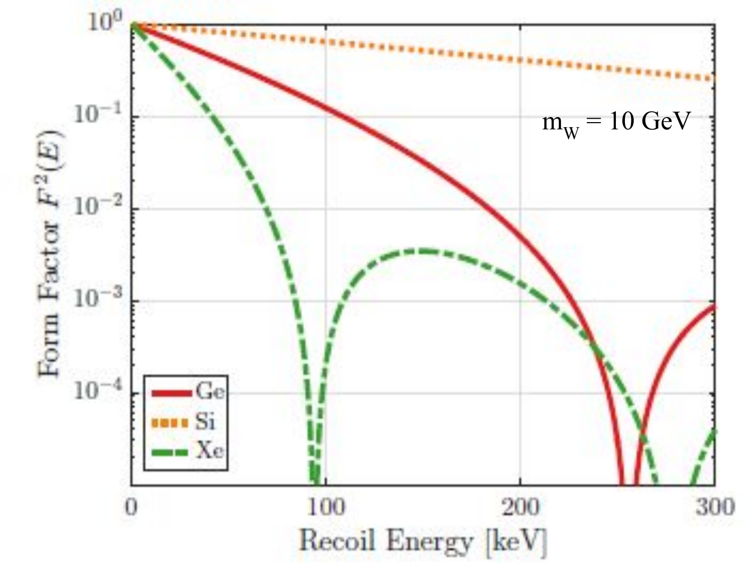
Precise crystal orientation, machined and polished dimensions

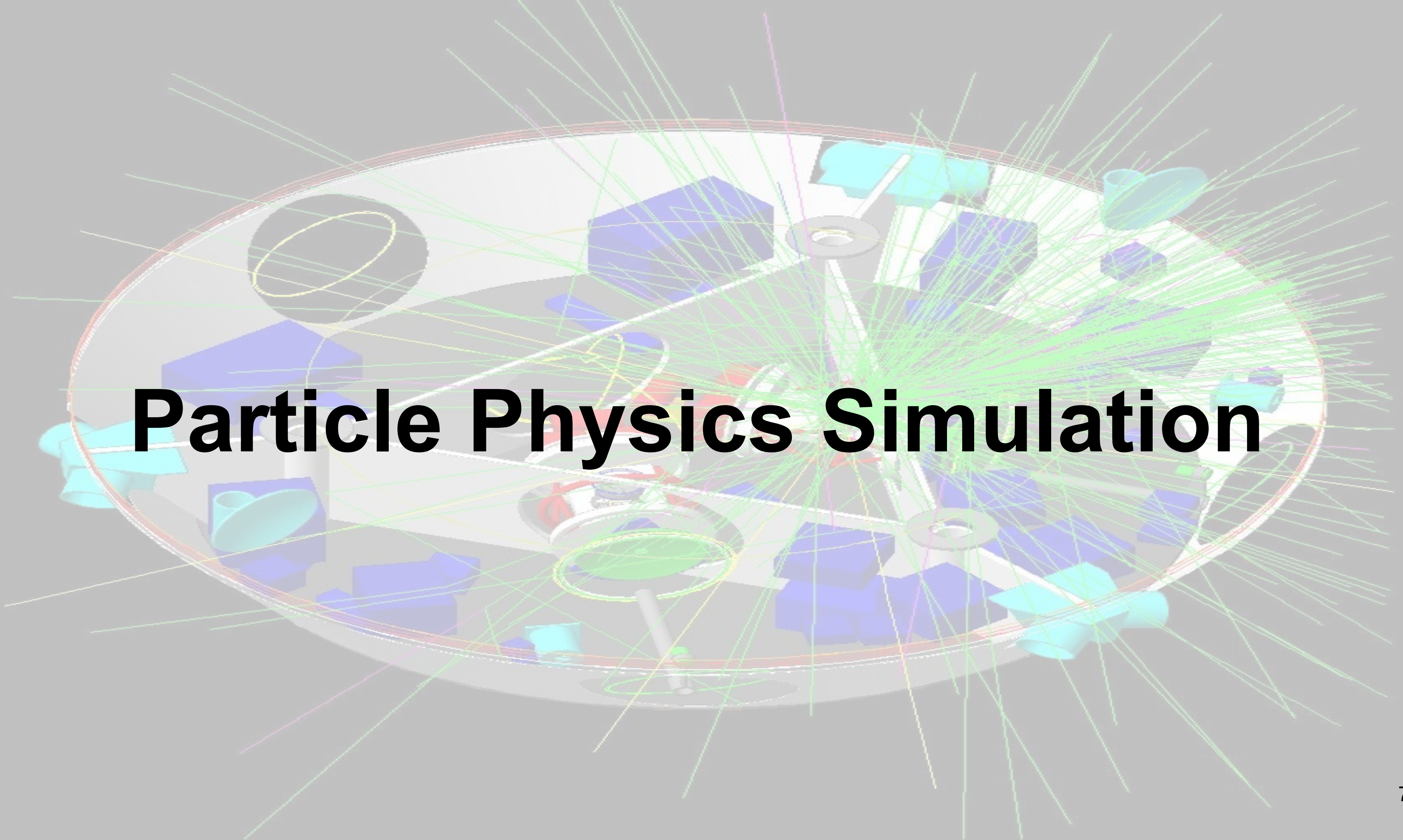
Some germanium, some silicon

- Different atomic masses will produce different recoil signals
- Protons vs. neutrons, nuclear spin, may be sensitive to specific theoretical interactions

Cooled to 50 millikelvins

- Suppresses thermal noise
- Sensors and readout superconducting





Particle Physics Simulation

What Does Geant4 Do?

Particle transport through materials, interactions of particles with atoms ("EM processes") or nuclei ("hadronic processes")

Processes implemented for energies ~100 eV to ~10 TeV

Particles tracked until all energy lost (e.g. through dE/dx), or decay

Transport assumes simple relativistic kinematics ($E^2 = p^2 + m^2$)

Transport in electric, magnetic fields handled with user-written functions to define field shape, extent

Geant4 and “Detector Backgrounds”

Geant4 models particle transport through materials, and interactions with atoms (“EM processes”) or nuclei (“hadronic processes”)

Many natural sources of radiation are “backgrounds” to signals of interest; artification sources can be used for detector calibration

We define the full apparatus geometry in Geant4, and generate events with sources incident on apparatus and detector crystals

Interactions lead to energy deposited (**hits**) at locations in crystals

- EM interactions transfer energy to atomic electrons (ionization, dE/dx)

Example: Neutron Interactions in Crystal

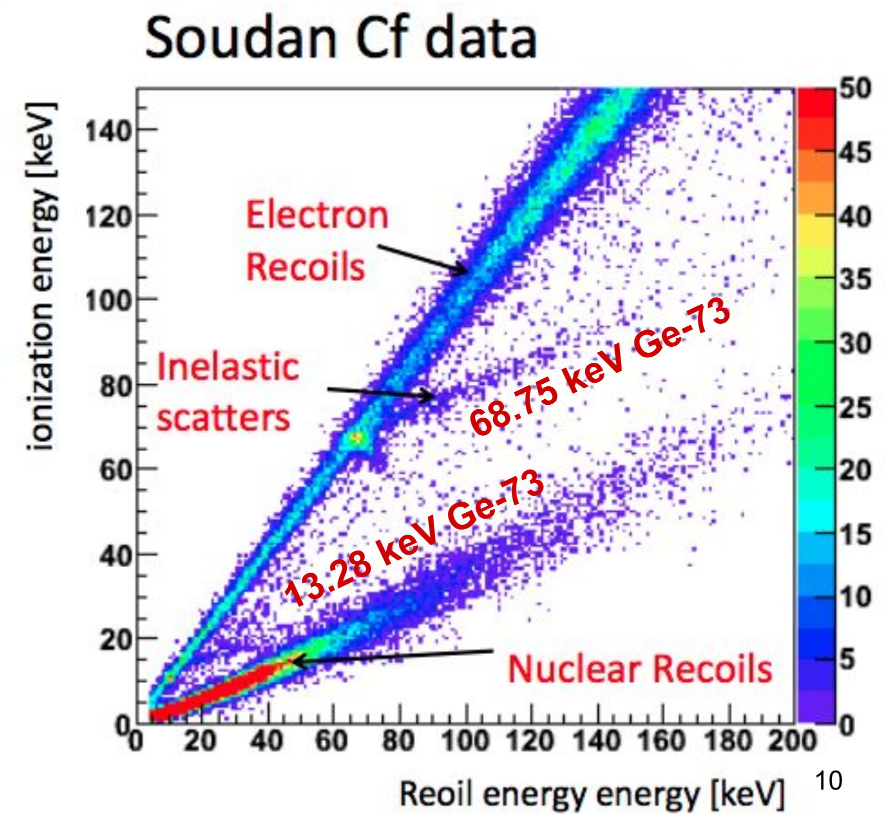
Neutron interactions are complex

- Simple elastic scatter, nuclear recoil
- Inelastic collision, excited nuclear state
- Neutron captures, induced radioactivity
- Multiple (~2.2) interactions per crystal

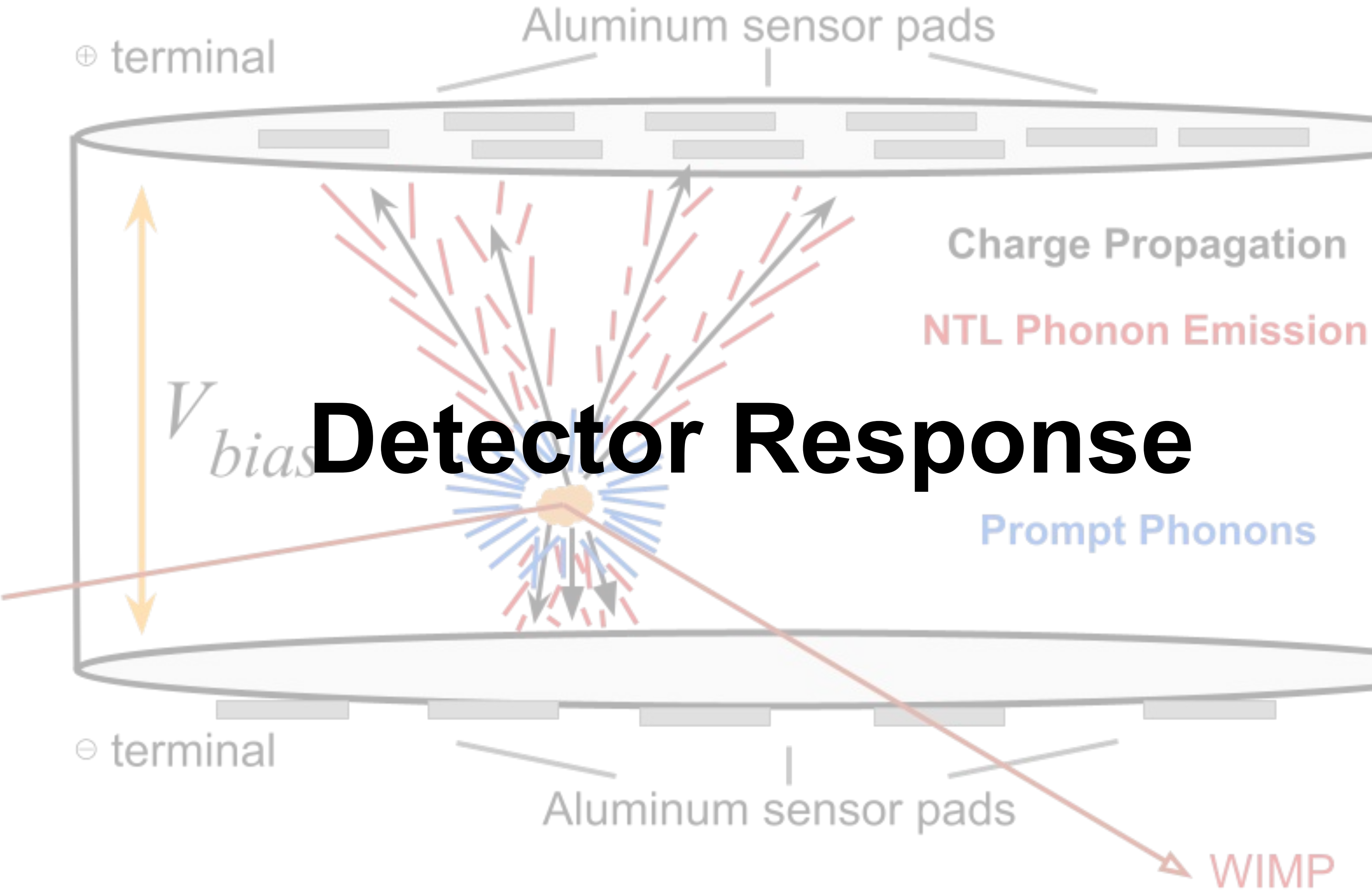
dE/dx vs. total energy has structure

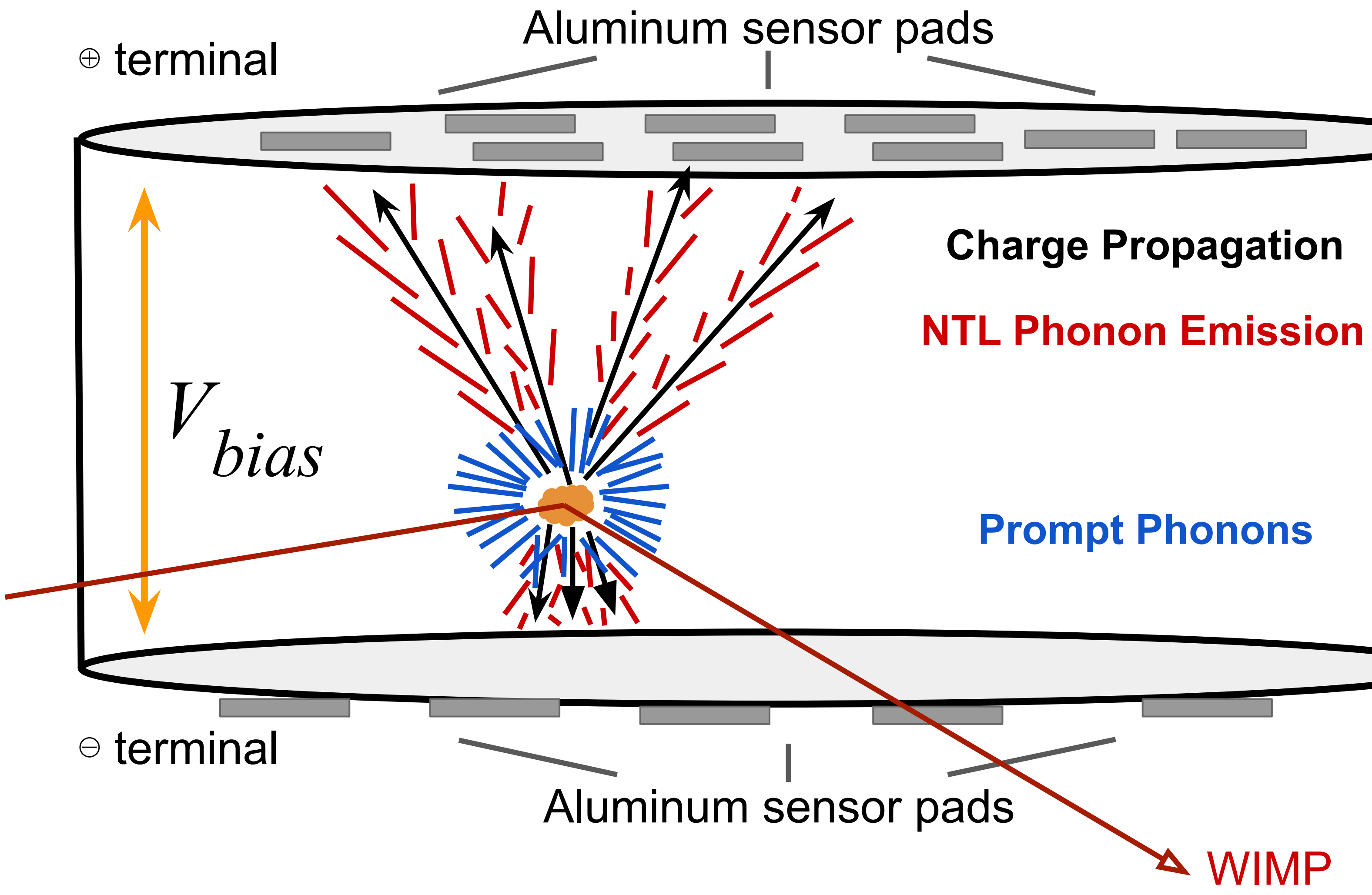
- **Electron recoils** are pure dE/dx
- **Nuclear recoils** are NIEL deposits
- Bands due to excitation gammas

Simulation reproduces Soudan data

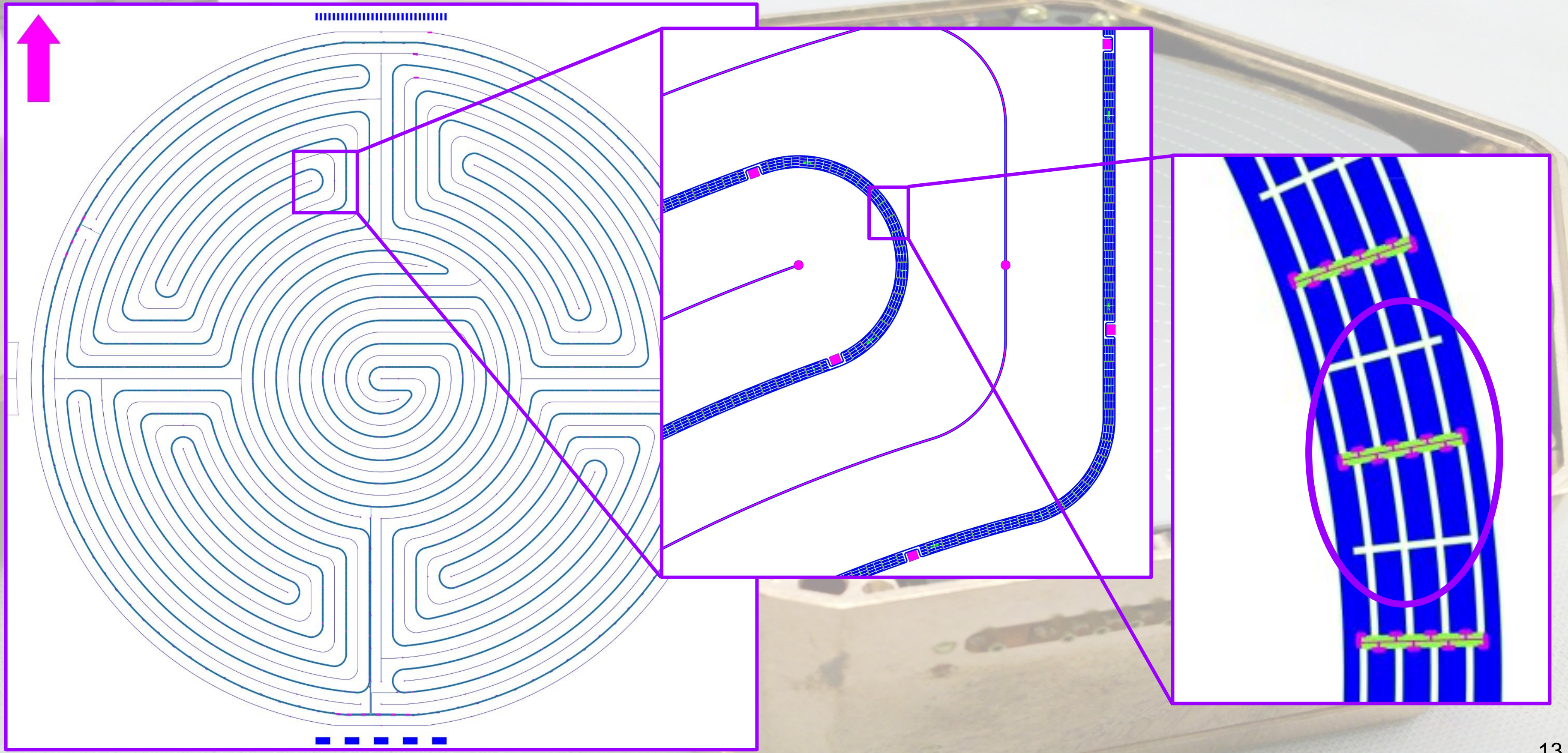


Detector Response




⊕ terminal
Aluminum sensor pads
Charge Propagation
NTL Phonon Emission
V_{bias}
Prompt Phonons
⊖ terminal
Aluminum sensor pads
WIMP

Detector Sensor Layout



SNOLAB iZIP7 with QETs

Charge Signals

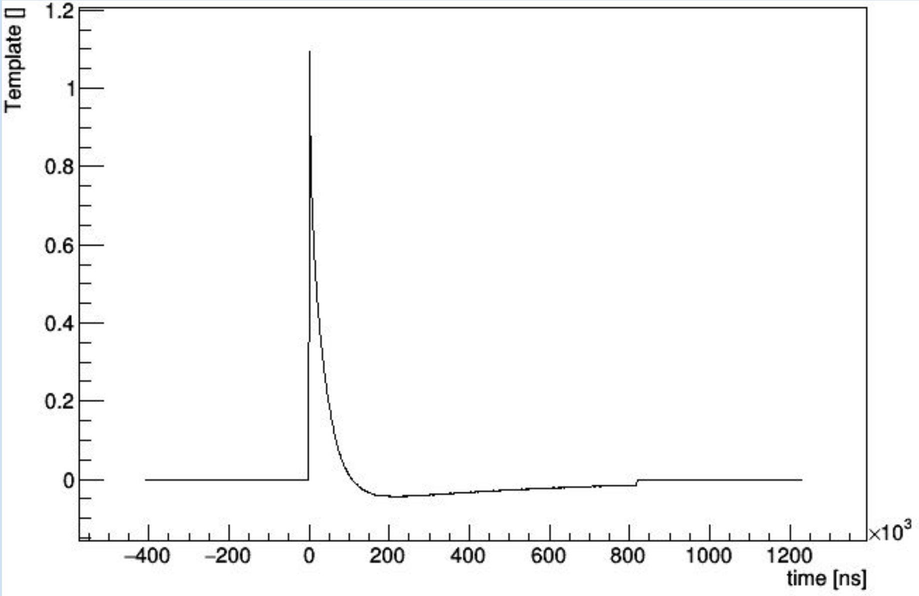
Particles incident on detector create electrons (-ve) and holes (+ve)

Voltage bias carries charges to electrodes on opposite sides

Spike proportional to total charge

Undershoot and tail due to readout circuit (RC components)

Crosstalk (+ or −) due to capacitance between channels



Phonon Signals

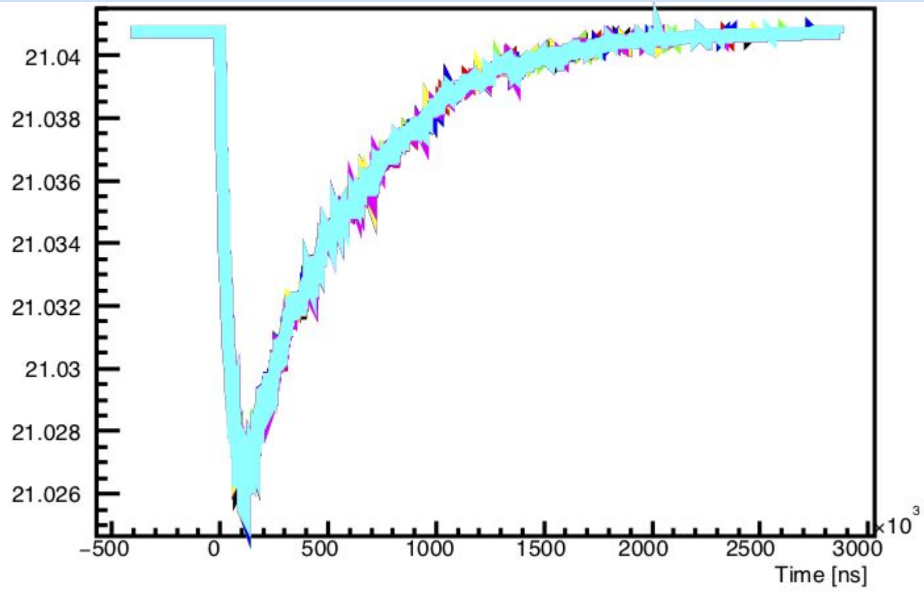
Charges gain energy in voltage, radiate phonons as they move

Phonons near surfaces arrive first, maxium when charges arrive

Long tail of late phonons “bouncing around” in detector

Integral measures total energy

Superconductor has less current when warm (after energy absorbed)



G4CMP: Geant4 Condensed Matter Physics

G4CMP : Condensed Matter Physics for Geant4

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

- Anisotropic transport of electrons
- Scattering, phonon emission (NTL), trapping

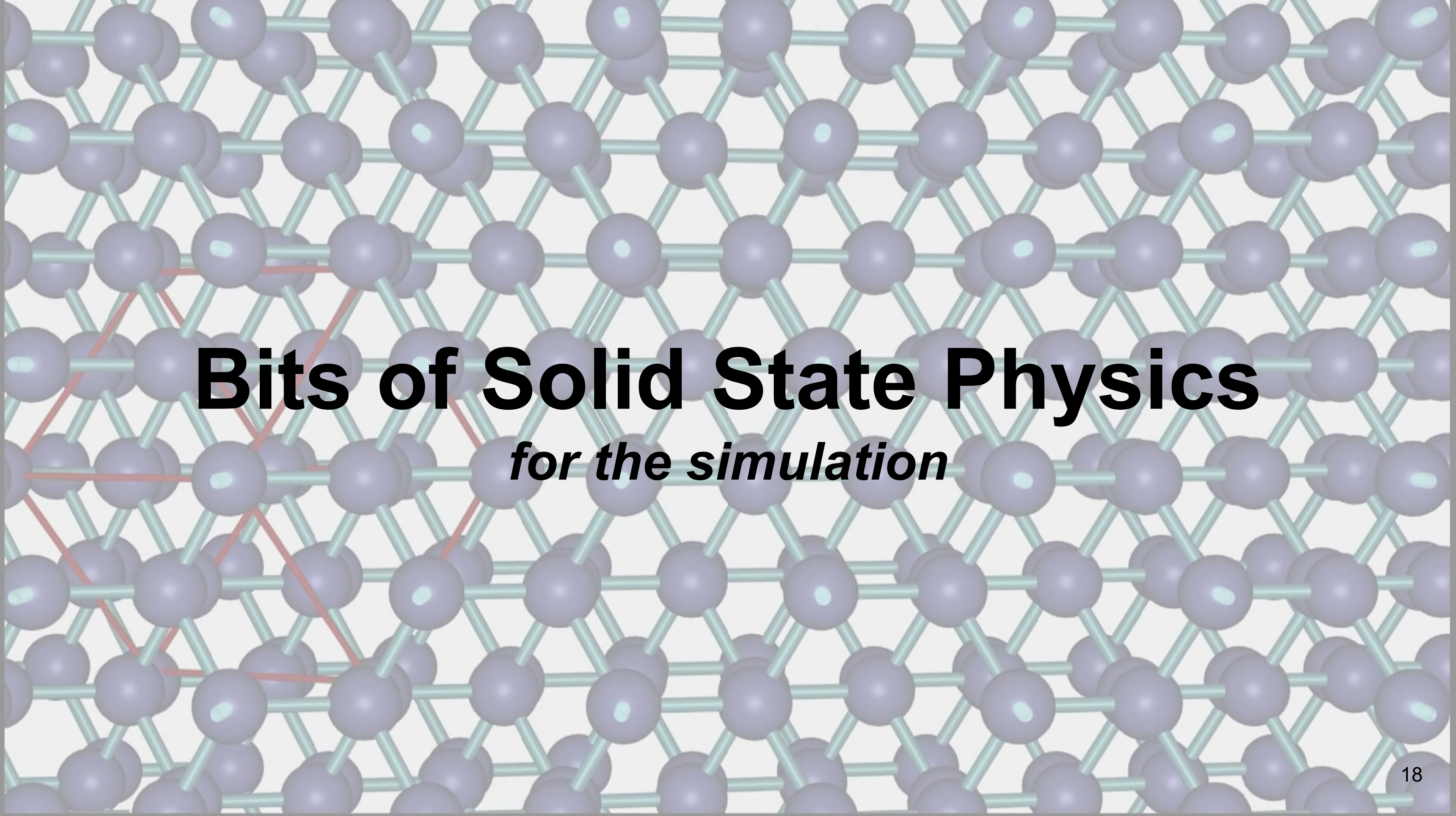
Transport of **meV-scale** (acoustic) **phonons** in deeply cryogenic crystals

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

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

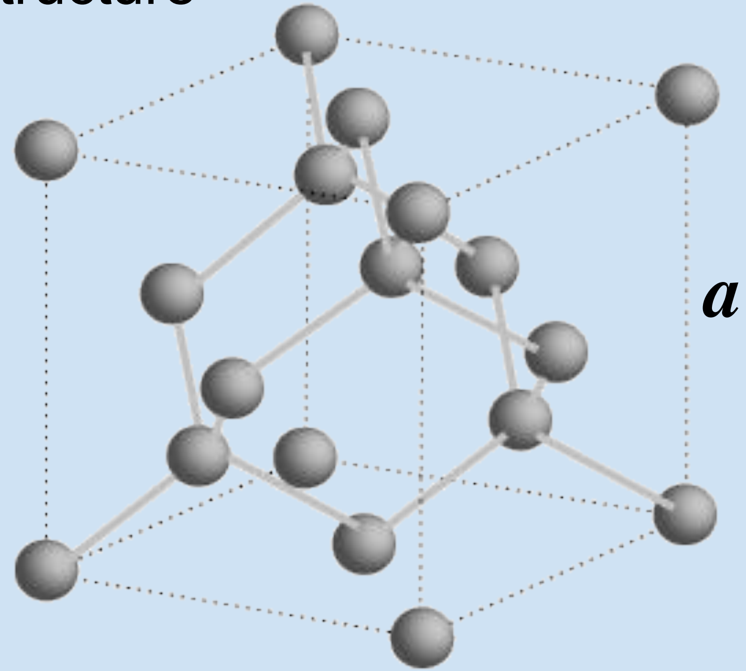


Bits of Solid State Physics

for the simulation

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

Charge Transport, Scattering and Valleys

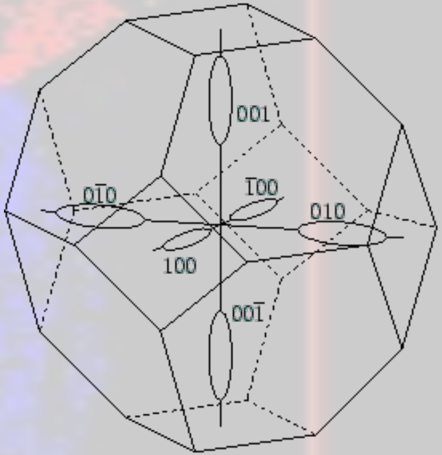
Incident particles promote electrons to conduction band, also creates holes (positive charge carriers)

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

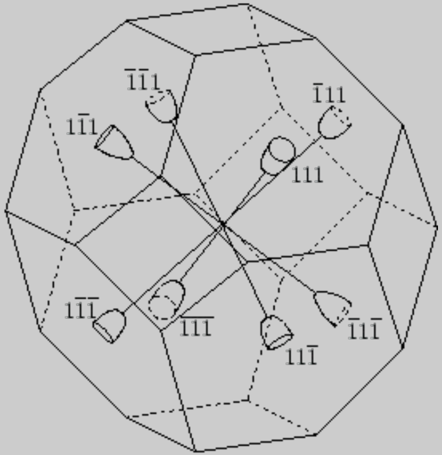
Electrons travel along valleys, with scattering between them

Charges accelerated in electric field radiate phonons

Charges interact with impurities, recombine with partner types



Silicon



Germanium

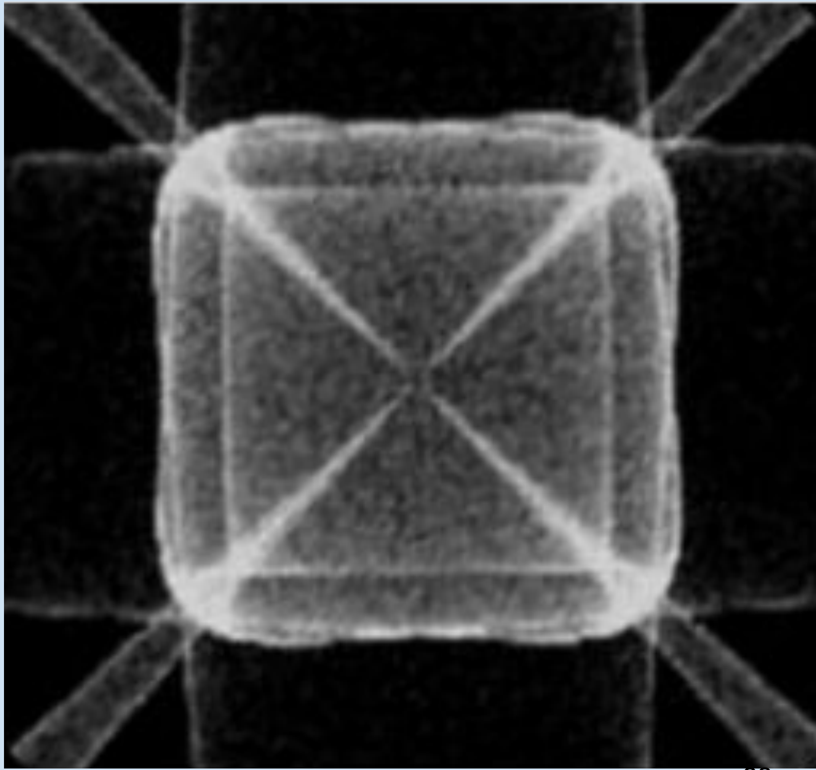
Phonon Transport

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



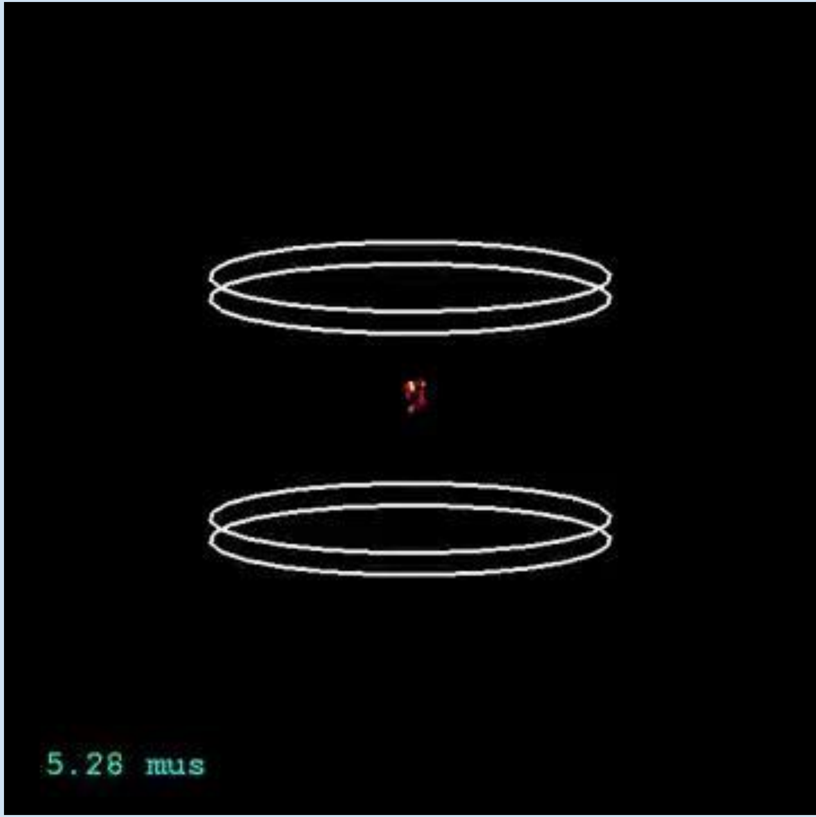
Phonons: Scattering and Equipartition

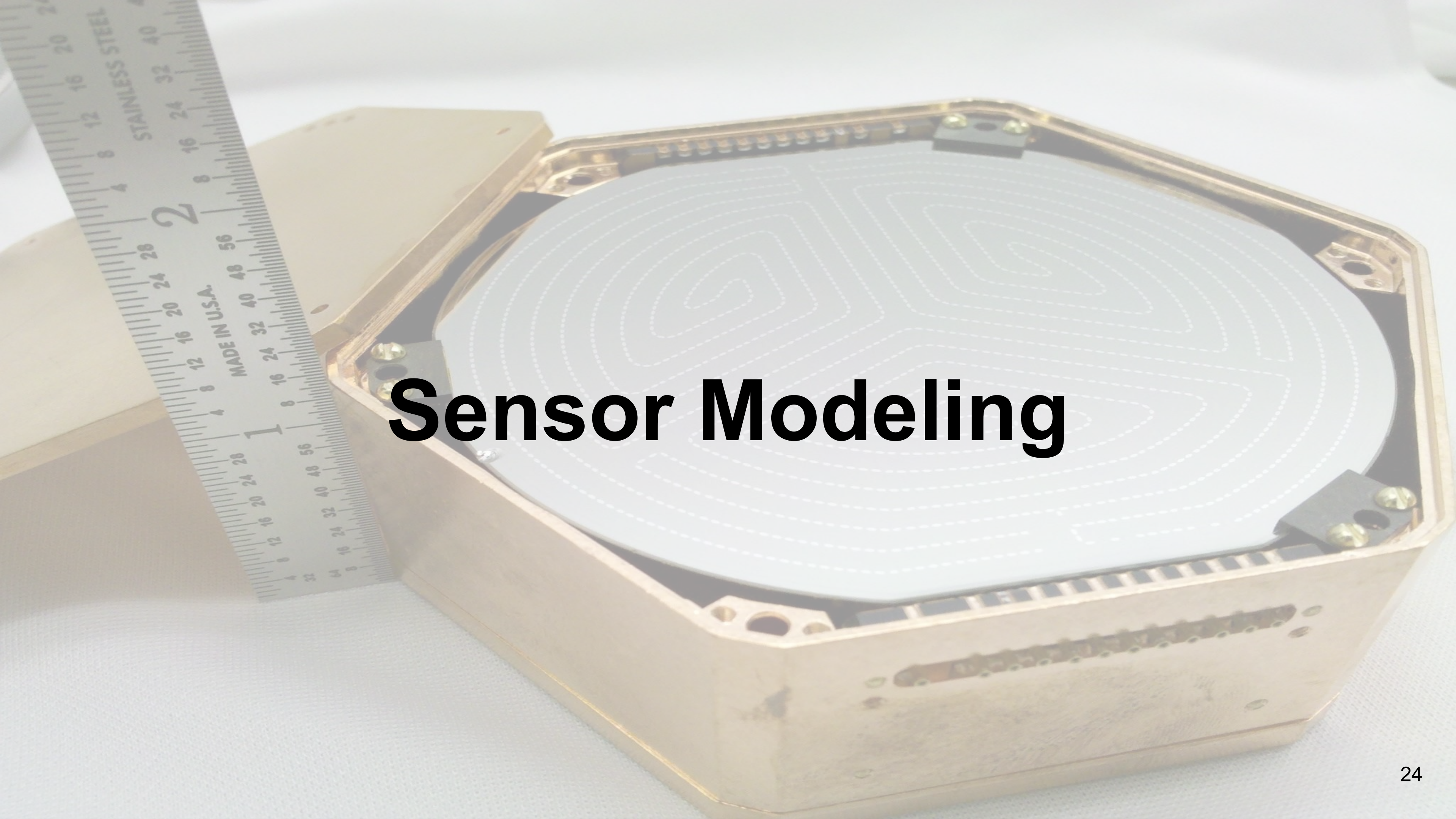
Higher energy (tens of meV) phonons scatter off of impurities, different isotopes, crystal defects

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





Sensor Modeling

QET: SuperCDMS's "enhanced" TES

***Q**uasiparticle trap assisted **E**lectrothermal feedback*
***T**ransition edge sensor*

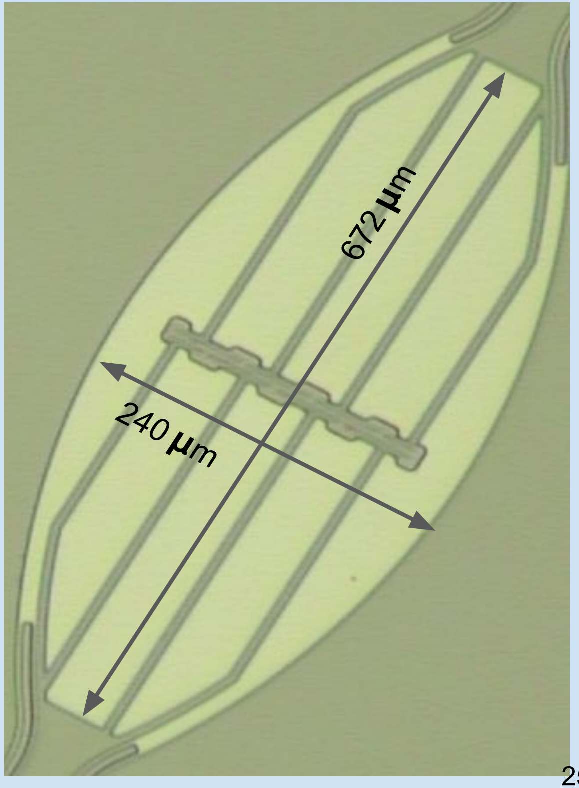
Absorbs phonons, produces change in current

Thin tungsten TES connected to readout lines

- On edge of superconducting transition
- Small δT ⇒ large δR ⇒ measurable δI

Attached to superconducting aluminum fins

- Phonons incident on Al break Cooper pairs
- Recombination re-emits phonons within Al



Phonon Signal Simulation

User application (SuperCDMS Sim) implements phonon collection

Geometry model includes QET pads on detector surface

Phonon incident on QET pad triggers thin-film simulation

- Phonon is killed by absorption
- Energy reported back from G4CMPKaplanQP as “absorbed” recorded as energy deposit (or “hit”) from incident phonon
- List of “re-emitted” or “reflected” energies become new secondary phonons

Considering moving to G4CMP, to make generally useful to users

Phonon Signals (Reprise)

Prompt and NTL phonons arrive quickly, max when charges stop

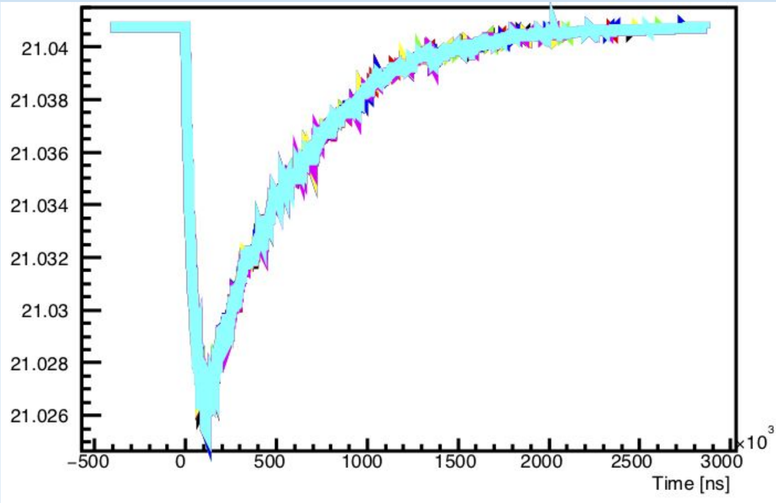
Downconversion, QET re-emission after prompt arrivals

- Long tail of low energy phonons,
- Several milliseconds to collect

Integral measures total energy deposit

Peak can be used as proxy as well

Superconducting sensor has less current when warm (after energy absorbed)

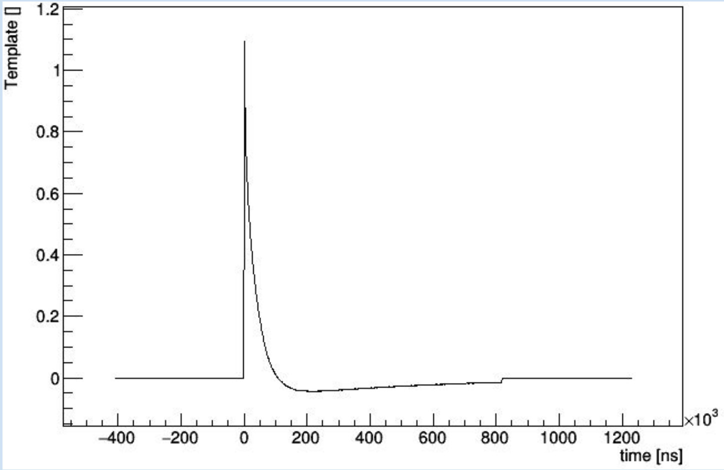


Charge Signals (Reprise)

User application (SuperCDMS Sim) implements charge collection

Shockley-Ramo theorem: induced current $i = q\,\mathbf{\hat{E}} \cdot \mathbf{v}_q$, $q = \pm 1$

- Special field $\mathbf{\hat{E}}$: signal electrode 1V, others 0V
- Charges travel much faster than DAQ readout (20-30 km/s, about 1 μs across detector)
- Path integral, $Q_{\mathrm{ramo}} = q \cdot V_{\mathrm{ramo}}$
- Sum over all charges, for all electrodes



Model circuit elements, capacitance matrix

Signal amplitude proportional to total charge, tail due to electronic response (RC circuit)

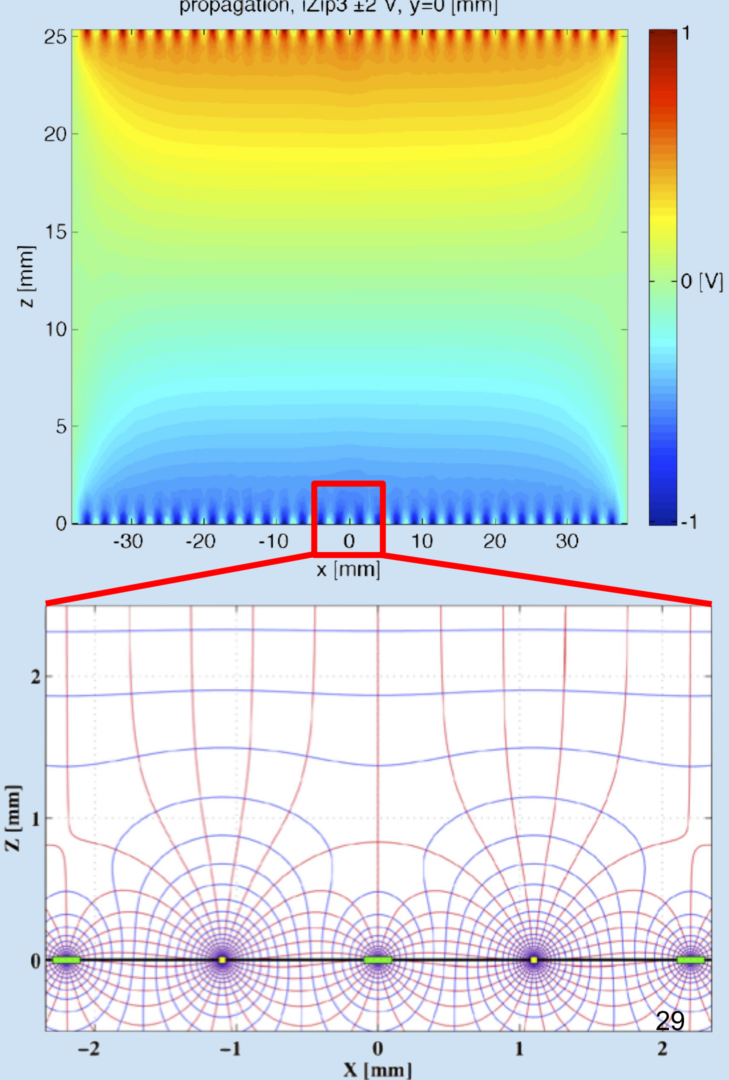
Finite Element Electric Field

Large detectors can have complex shapes and electrode layout

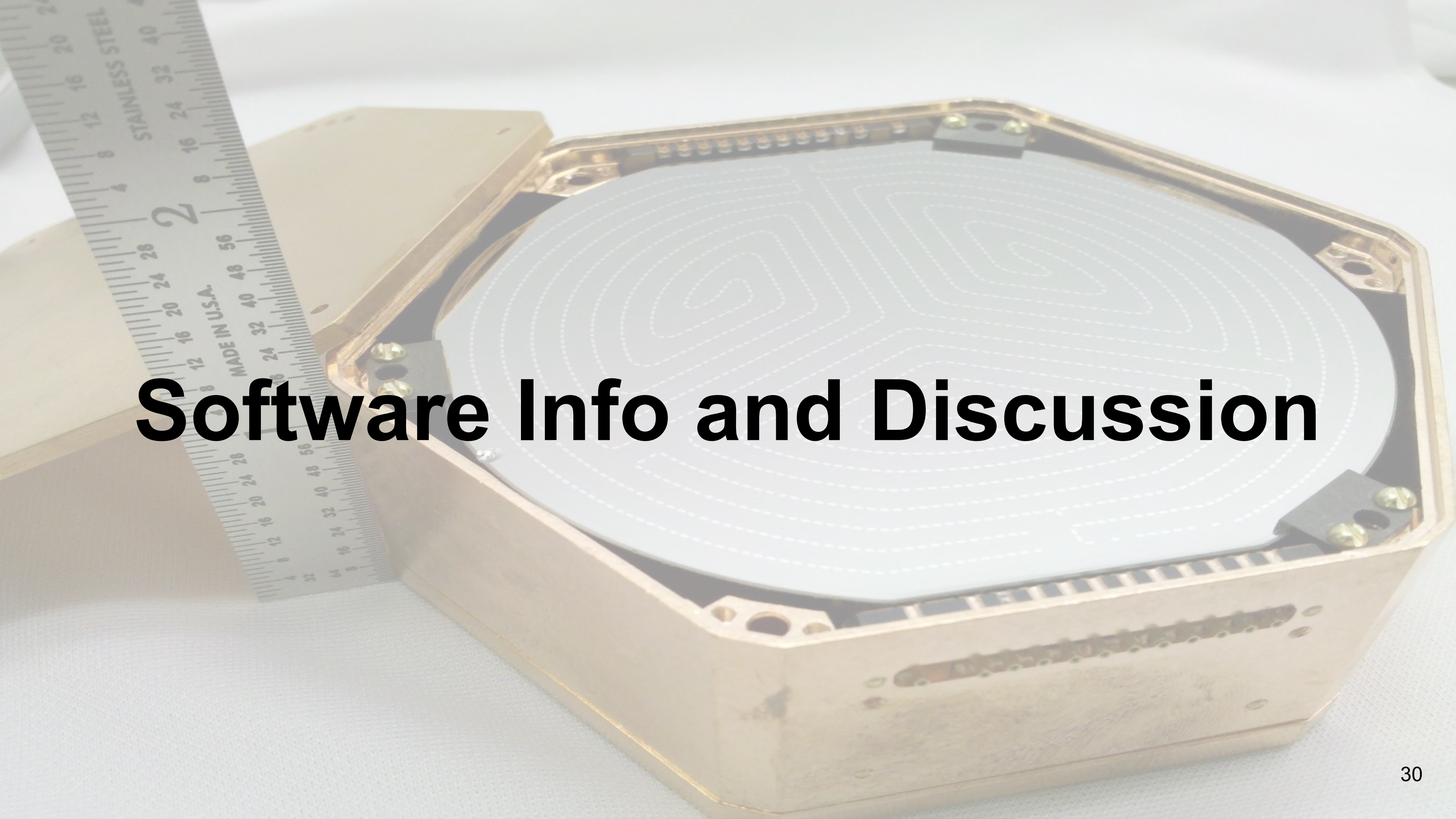
COMSOL, FEniCS, other physics modeling packages can generate a tetrahedral mesh of voltage at coordinates

G4CMPTriLinearInterp processes table of mesh points, tetrahedra

G4CMPLocalElectricField handles mesh in detector-local coordinates



Software Info and Discussion



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)

Descriptive paper: arXiv:1403.4984 (preprint only)

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

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)

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

No peer-reviewed publication

No public issue tracking: using CDMS-internal JIRA tracker

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

Summary

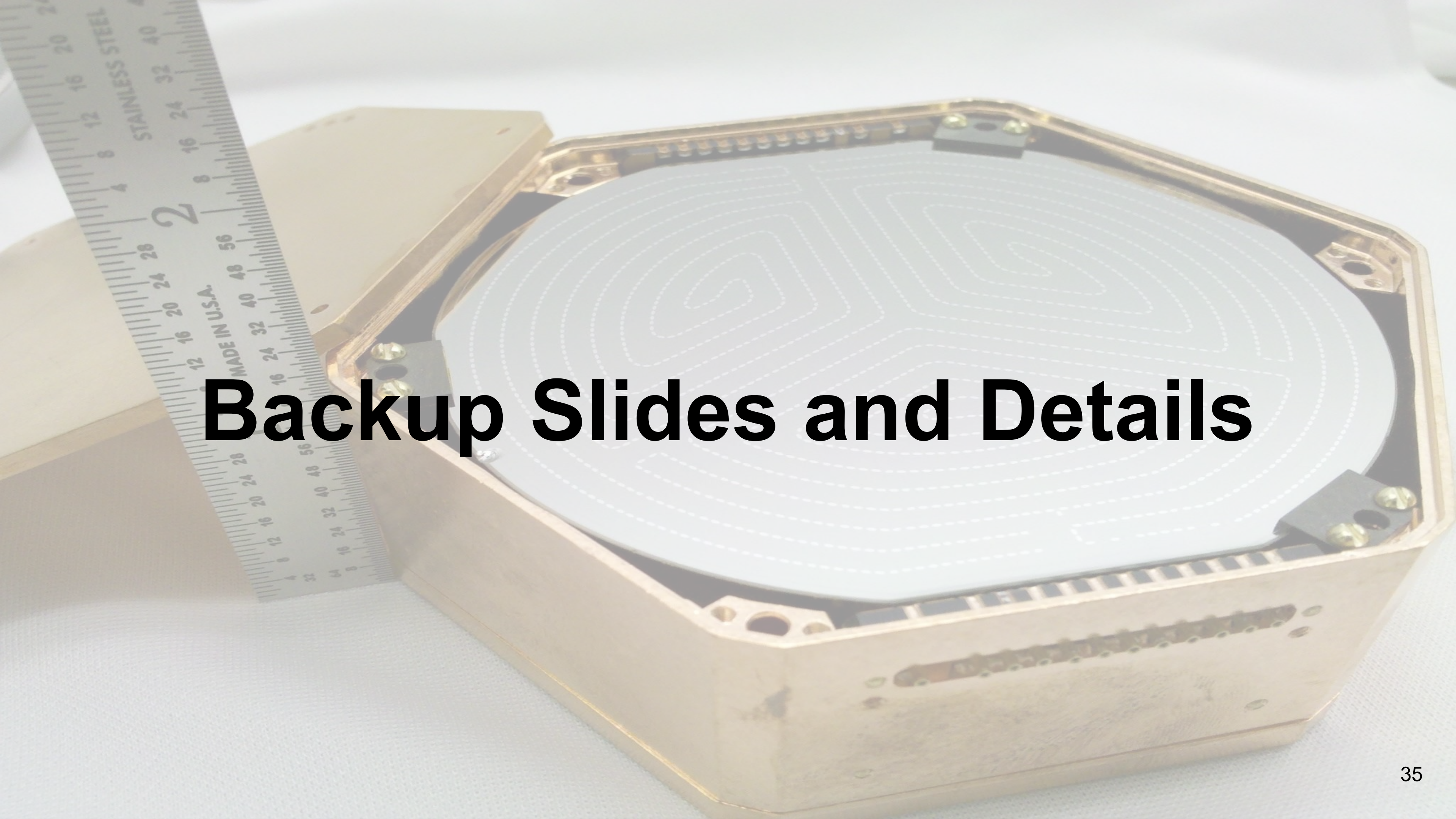
G4CMP provides a detailed "micro" simulation of detector response in cryogenic semiconductor crystals

Integrated with Geant4 HEP simulation toolkit

Simulates SuperCDMS detectors with detailed readout signals

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)
valley   0  0  0 deg
valley   90 90 0 deg
valley   0 -90 -90 deg
```

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 $\vec{x}$, then $\underline{\underline{\mathbf{m}}} = \begin{bmatrix} m_{/\!/} & 0 & 0 \\ 0 & m_\perp & 0 \\ 0 & 0 & m_\perp \end{bmatrix}$, $\vec{p} = \underline{\underline{\mathbf{m}}}\,\vec{v}$, $E = \vec{p}^T\,\underline{\underline{\mathbf{m}}}^{-1}\,\vec{p}$

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

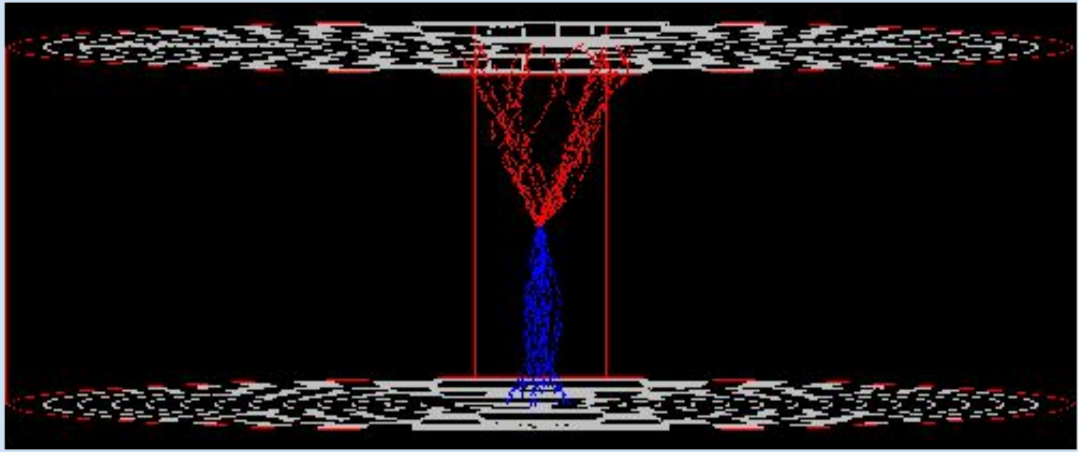
Electrons may be strongly scattered by absorption of thermal phonons

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**



Neganov-Trofimov-Luke Phonon Emission

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

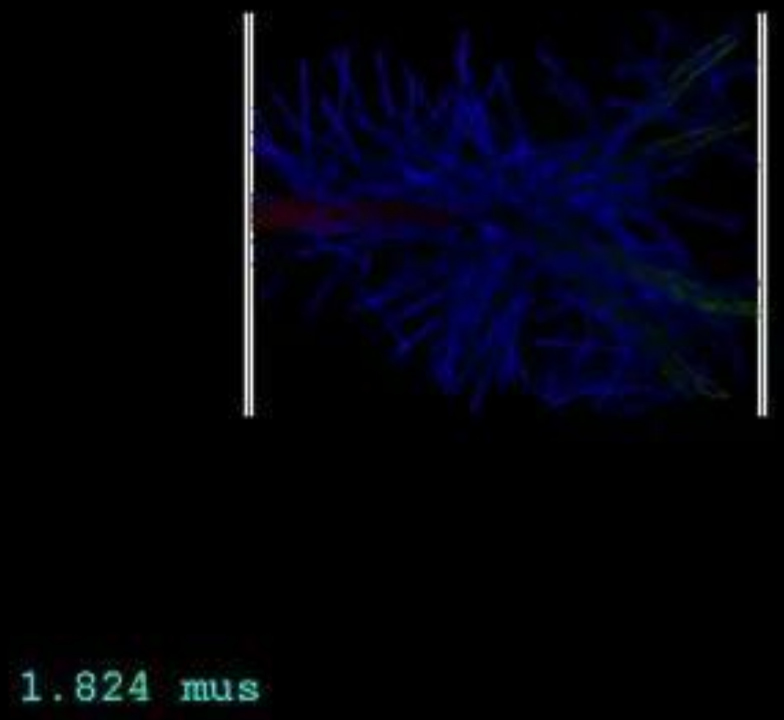
Interact with lattice to radiate phonons, reducing energy and changing direction

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

Total phonon emission equals energy gained from potential

G4CMPLukeScattering

G4CMPLukeEmissionRate



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

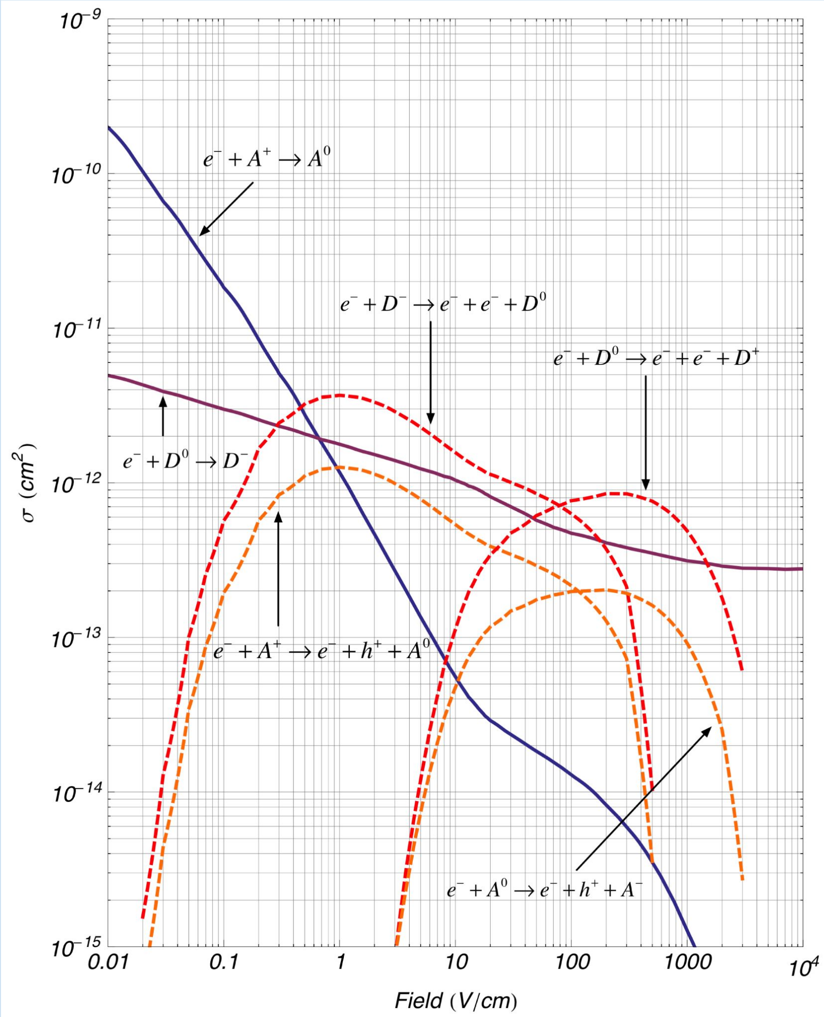
Two impurities, four kinds of reionization, with separate rates

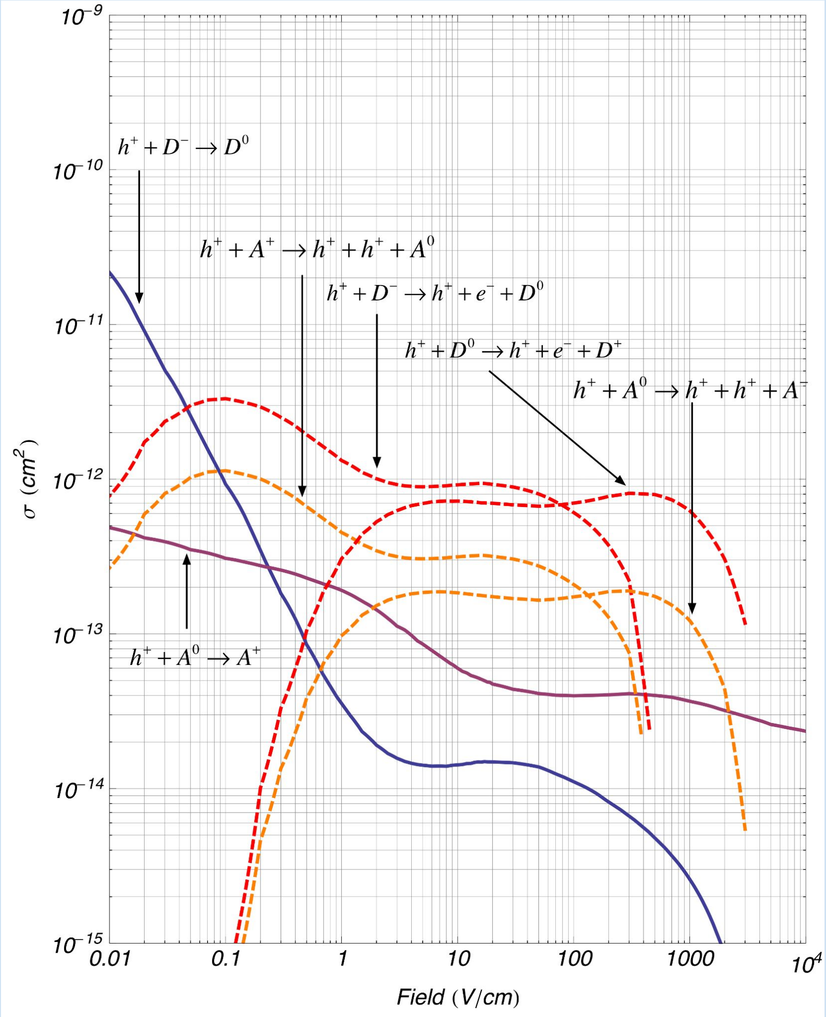
- $e + D^{-} \rightarrow 2\,e + D^{0}$, $e + A^{+} \rightarrow e + h + A^{0}$
- $h + A^{0} \rightarrow 2\,h + A^{+}$, $h + D^{-} \rightarrow h + e + D^{0}$

G4CMPDriftTrapIonization

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

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


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


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

Phonon Mode Group Velocity

Use crystal stiffness matrix along a given direction **n̂**

- 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 **n̂** 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: $\nu = B \cdot (E/h)^4$

- $B = 2.43 \times 10^{-42}\ s^3$ (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: $\nu = D \cdot (E/h)^5$

- $D = 2.43 \times 10^{-42}\ s^3$ (Si), TT / L’T fraction 74% (Si)

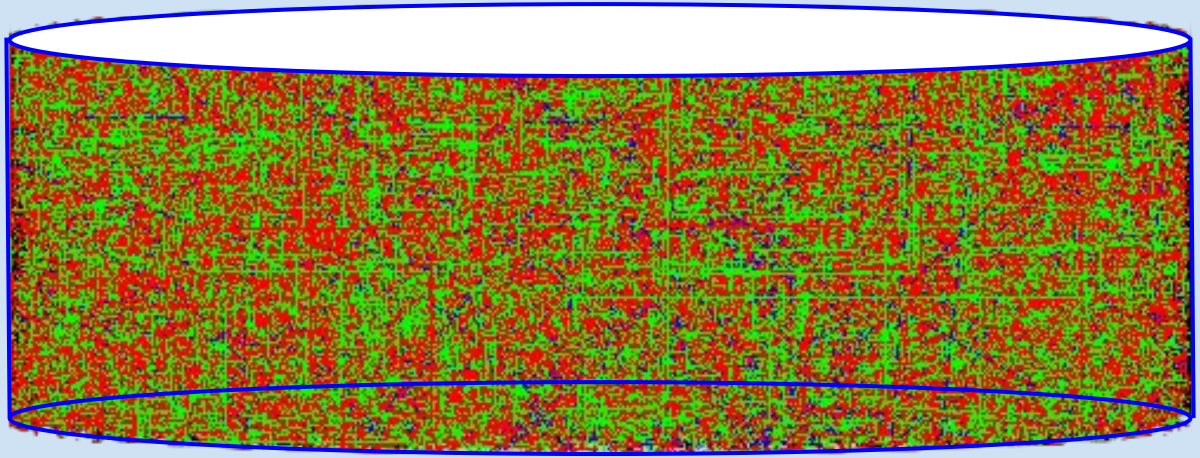
Equipartitions early “hot” (Debye energy, tens of meV) phonons into sea of meV-scale phonons

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



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)

Lindhard/Robinson or Lewin/Smith Partition

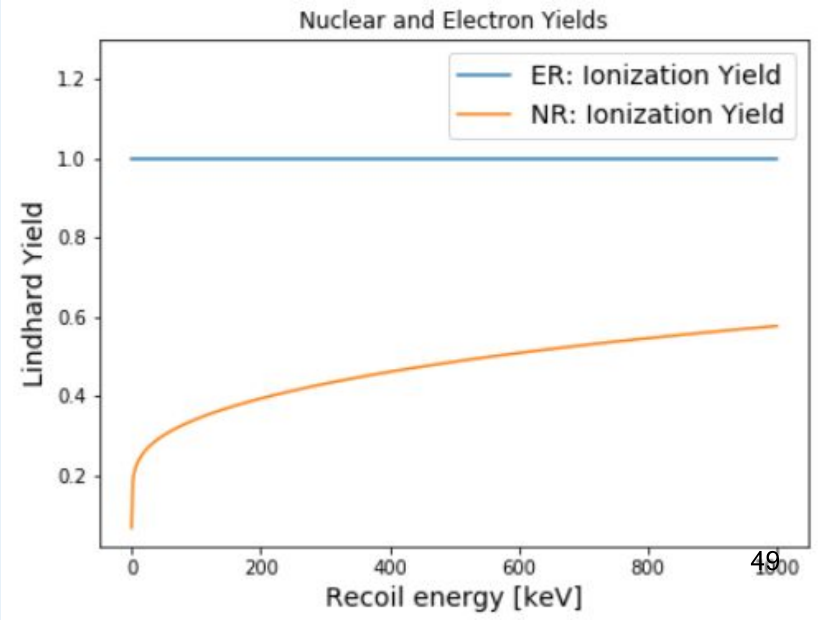
Relative magnitude of dE/dx vs. NIEL for ions depends on charge and mass of projectile, and atomic number and mass of crystal atoms

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



Kaplan Quasiparticle Model

Thin-film superconductors common in cryogenic electronic sensors

- TES/QETs, KIDs, qubits

Populated with Cooper pairs

- Phonon absorption can break pairs into electron quasiparticles
- For small films, quasiparticle transport faster than thermal response

Model energy transfer, QP transport, phonon re-emission

Aluminum film parameters supplied via G4 “properties table”

- Film thickness, Cooper pair gap energy (2Δ), v_{sound}, phonon lifetime

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
- $P = \exp(-4d/MFP)$ $\quad$ $MFP = v_{sound}/\boldsymbol{\tau}(E)$ $\quad$ $\boldsymbol{\tau}(E) = \boldsymbol{\tau}_0 / (1 + \delta\boldsymbol{\tau} \cdot (E/\Delta - 2))$

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 absorber

Phonon Readout Model

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.