Crystal physics and phonon transport in Geant4

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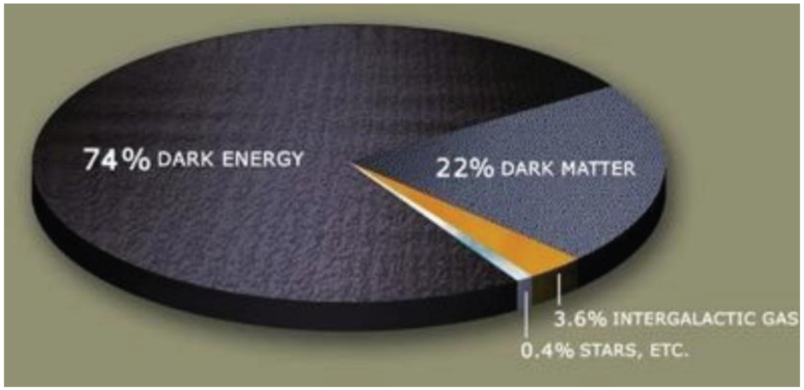
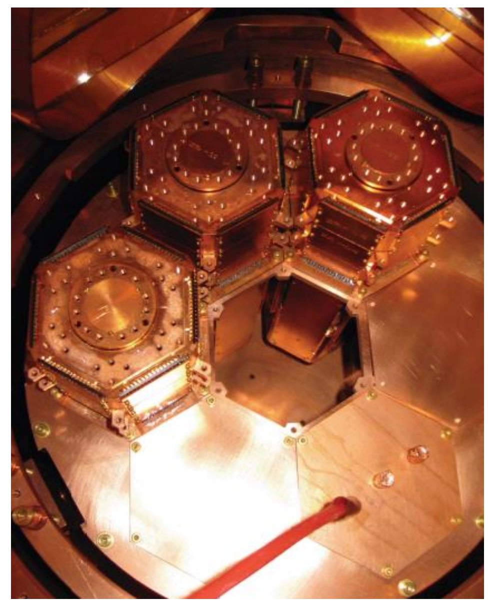
The Cryogenic Dark Matter Search (CDMS)



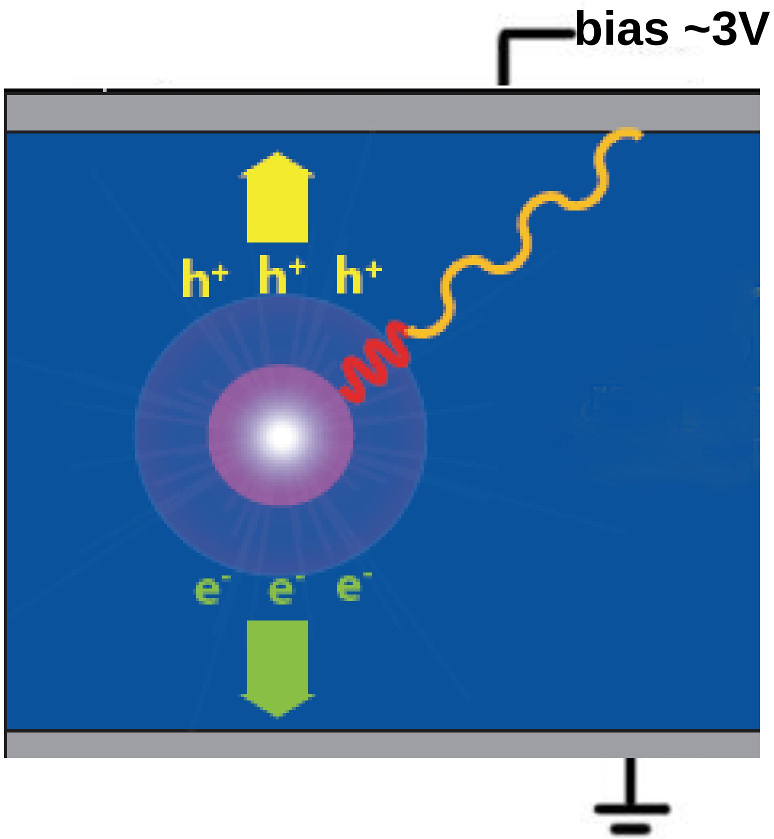
- The majority of the mass energy in the Universe is dark matter
  - » No EM interaction
  - » Gravitational interaction
  - » Non-baryonic



- CDMS attempting to detect WIMP interactions with crystals
- Deep underground
  15kg Ge@50mK
- Pretty much opposite of a space application

Motivation: SuperCDMS Detector Monte Carlo

- A particle scattering in a crystal will create both phonons and electron-hole pairs
- Electron-hole pairs are collected by a small drift field
- Phonons are collected by Transition Edge Sensors (TESs)

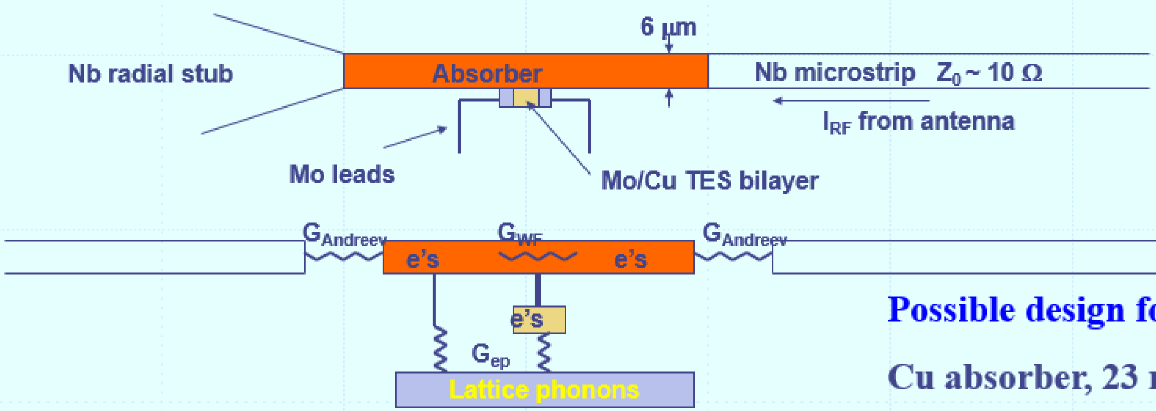


Deposited by WIMP: 10-100 keV
e-/hole pair: 3 eV to create
Individual phonon: ~80 meV to create

Motivation: Community interest

- Not just relevant to CDMS...
  - Neutrinoless beta decay
    image from www.lngs.infn.it

Other dark matter searches *image from cresst.de*



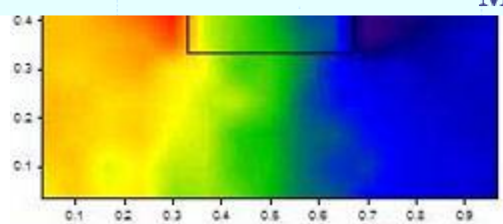
Taken from Ali et al., Univ. Wisconsin

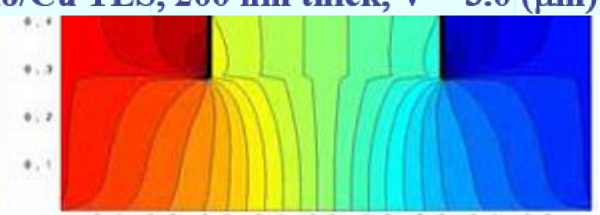
Possible design for low-background CMB observations:

Cu absorber, 23 nm thick, V = 6.2 (μm)^3

R = 10 W

Mo/Cu TES, 200 nm thick, V = 3.0 (μm)^3

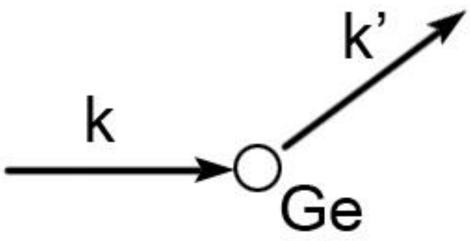




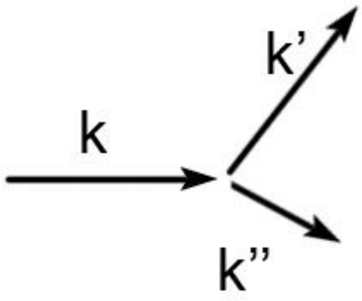
Physics processes

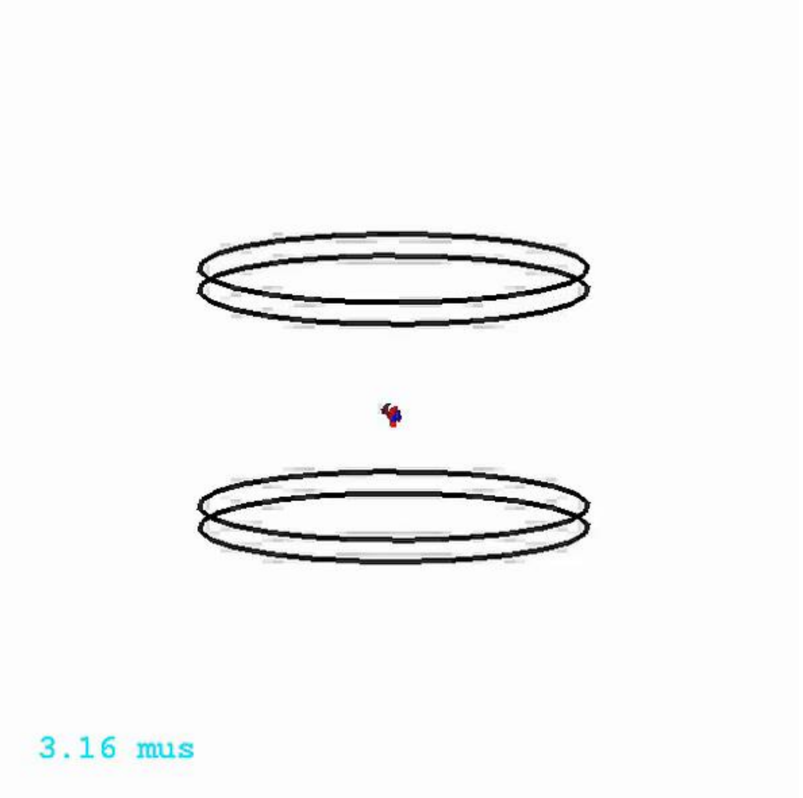
The CDMS detectors operate at 40 mK . Two phonon processes are relevant.

1) Isotope scattering and mode mixing



2) Anharmonic down conversion





Physics processes

- Isotope scattering and mode mixing

```
XPhononScatteringProcess : G4VDiscreteProcess
```

- Anharmonic downconversion

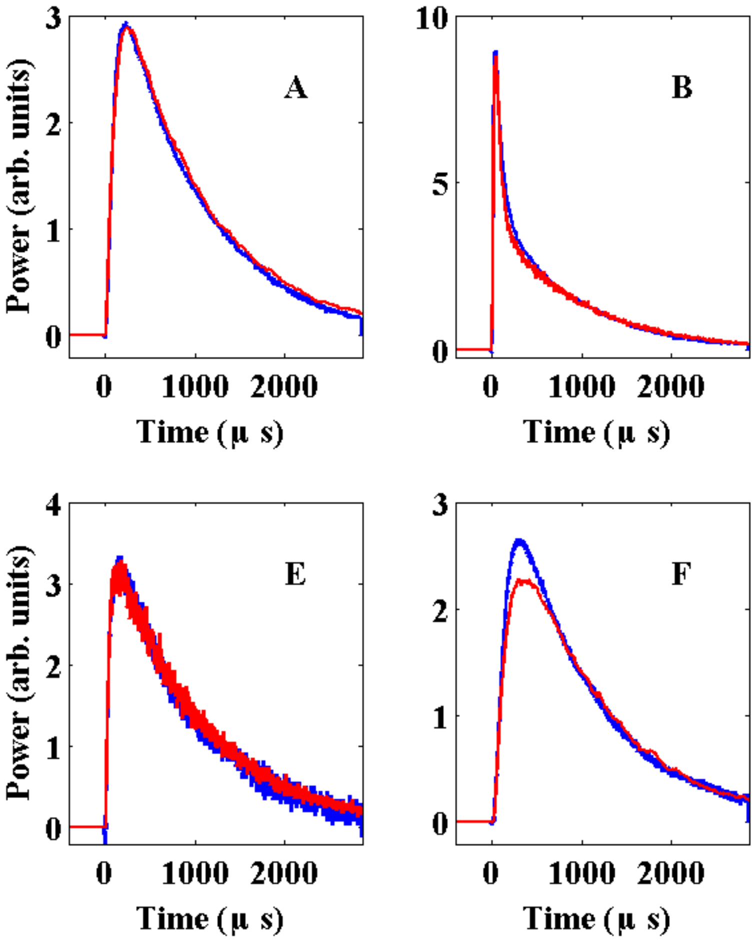
```
XPhononDownconversionProcess : G4VDiscreteProcess
```

- Phonon focusing using singleton lattice manager object

XLogicalLattice(*dynamic constants*)
XPhysicalLattice(&XLogicalLattice, *orientation within volume*)
XLatticeManager3::registerLattice(&G4VPhysicalVolume,
&XPhysicalLattice)

Simulating the CDMS Signal

- Simulated phonon pulse shapes match well with observed pulse shapes
- Pulse shapes shown are simulated TES traces
- TES simulation currently performed in matlab
- Matlab provides output in CDMS-raw format



Real (blue) and simulated (red) phonon pulses, matlab. *Image produced by Leman et al.*

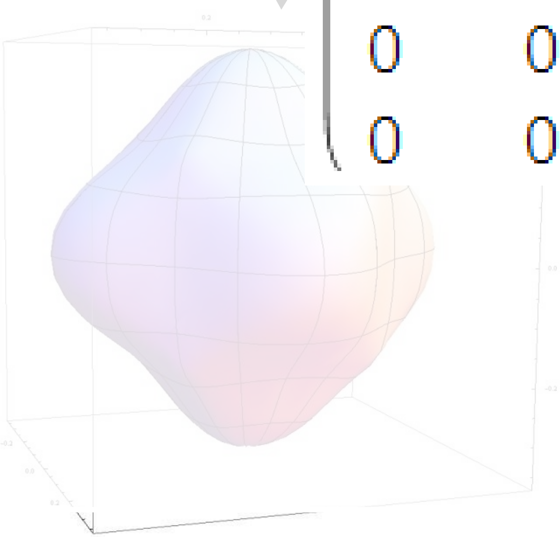
Phonon focusing

$$[C_{ijml} n_j n_l / \rho \quad - v^2 \delta_{il}] e_l = 0$$

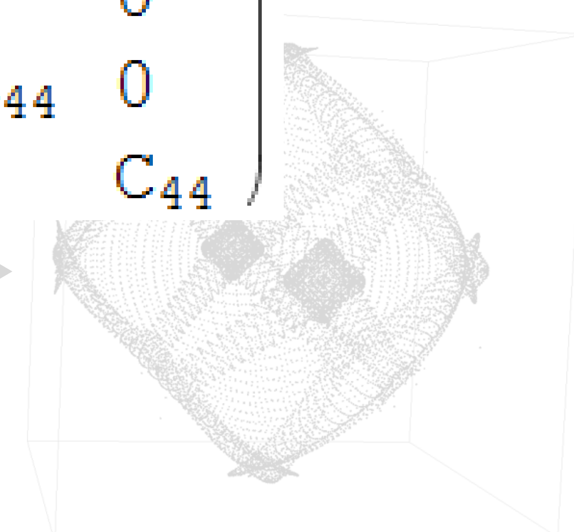
n=wave vector direction
v=phase velocity
e=polarization vector
ρ=local mass de

- In order to generate focusing effect, solve 3d wave equation
- Contracted elasticity tensor likely has ~3 independent components

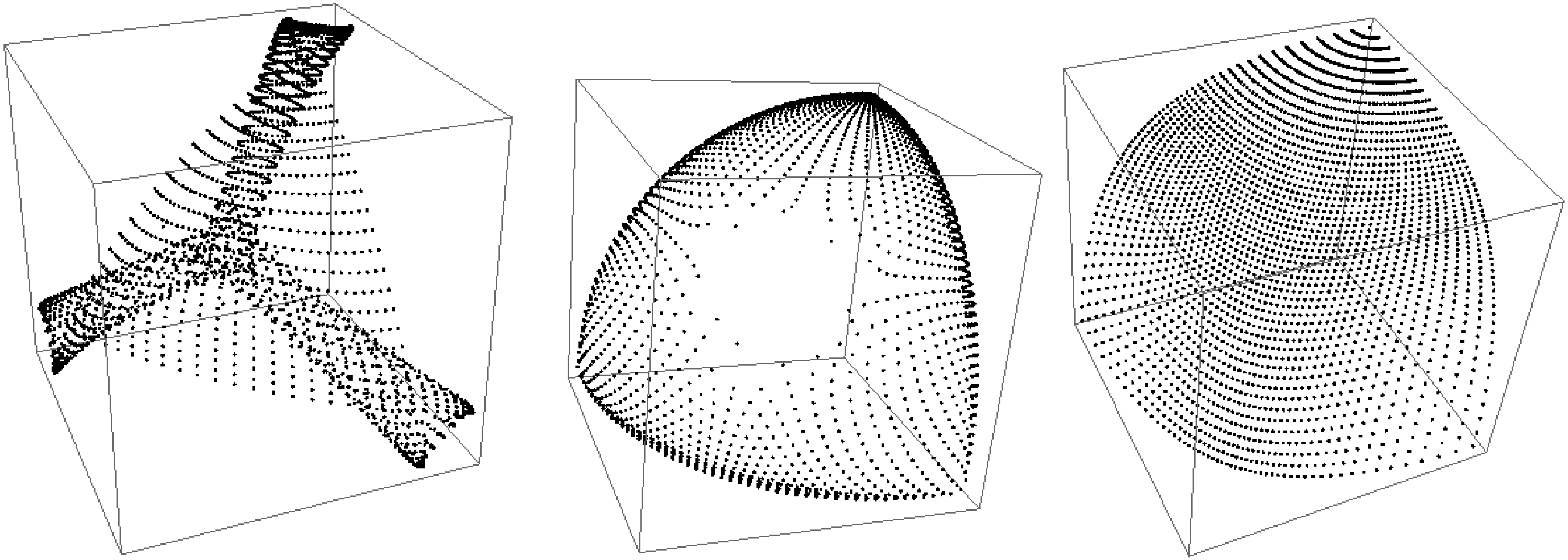
$$\begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$



Gradient of slowness surface yields group velocities



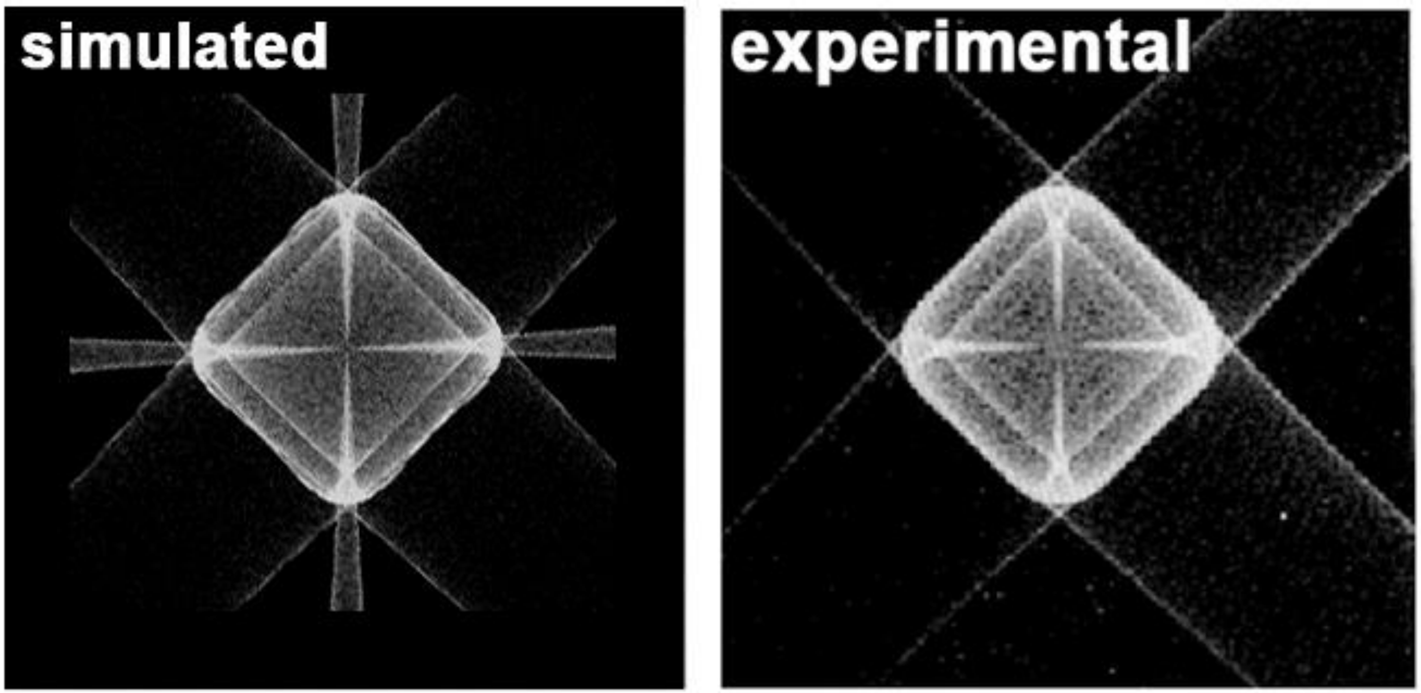
Group velocity densities



- **Densities of group velocity vectors, left to right:** Longitudinal, slow transverse, fast transverse

Phonon caustics in Germanium

- Anisotropies in the elasticity tensor cause phonons to be focused onto preferred propagation vectors.



*Phonon flux intensity on a Ge crystal face due to a point source at the crystal center. **Left:** simulated with Geant4 **Right:** as observed by Nothrop and Wolfe*

Phonon example in Geant4 v9.6

- Phonon transport code available as example since v9.6.0

```
examples/extended/exoticphysics/phonon
```

- In its current form the example stores phonon arrival times/eneriges and xy locations in two .ssv files

```
examples/extended/exoticphysics/phonon/timing.ssv
examples/extended/exoticphysics/phonon/caustic.ssv
```

- The sort of caustics shown on the previous slide can be generated by reducing the initial phonon energy into the ballistic regime and creating a 2D histogram of *caustic.ssv*

Generating caustics using scorers - I

- Can use Geant4 scorers to create caustics. To enable scorers add the following to XGeBox.cc:

```
#include “G4ScoringManager.hh“
...
G4ScoringManager scoreMan = G4ScoringManager::GetScoringManager();
```

- Change the phonon energy in XPrimaryGeneratorAction:

```
void XPrimaryGeneratorAction::GeneratePrimaries(G4Event*)
        ...
        particleGun->SetParticleEnergy(0.0001*eV);
```

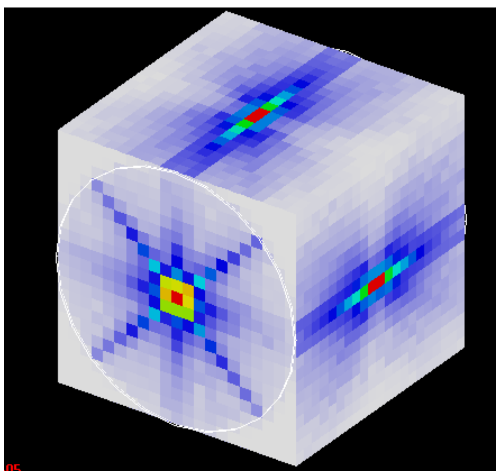
Generating caustics using scorers - II

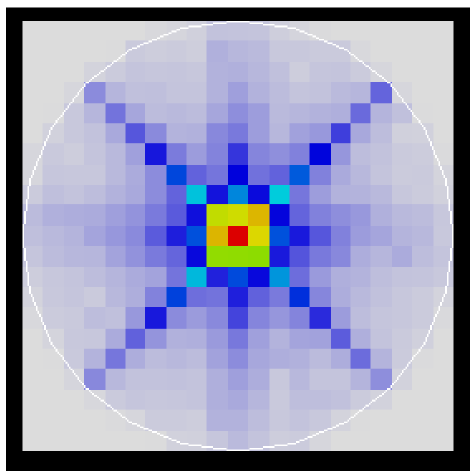
- Compile, run XGeBox and run the scoring script:

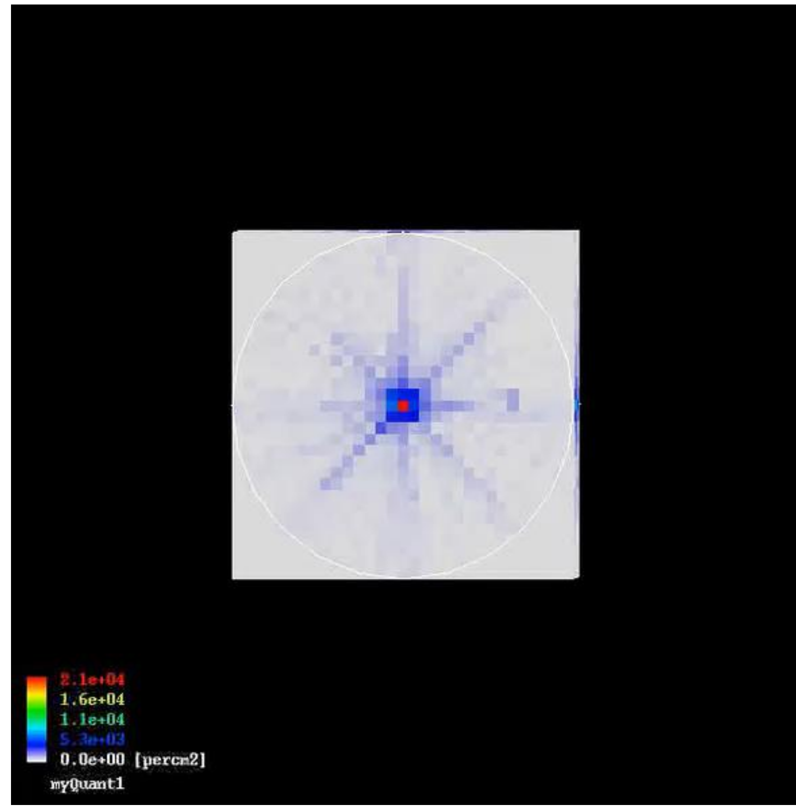
```
/score/create/boxMesh mesh1
/score/mesh/boxSize 0.01 0.01 0.01 m
/score/mesh/nBin 31 31 31
/score/quantity/flatSurfaceCurrent myQuant
/score/close

/run/beamOn 10000

/score/drawProjection mesh1 myQuant
```

Generating caustics using scorers - III

- These images were generated with the geant4 internal scorer outlined in the previous slide
- May need /scorer/colorMap/setMinMax







Conclusions

- Phonon transport at zero temperature implemented
- Phonon transport code available as example since v9.6.0
- Good agreement with experiment
- Can generate caustics using Geant4 scorers
- Can simulate any crystal whose elasticity tensor can be Voigt-contracted to 6x6 tensor
- Working on non-zero temperatures and optical phonons

Future Developments

- Generating phonons from physics processes
- Phonon transport at non-zero temperature
- Physical implementation of boundary interactions (including mode-matching for different crystals)
- Optical phonon processes
- Phonon transport in metals and semi-metals

The SuperCDMS collaboration

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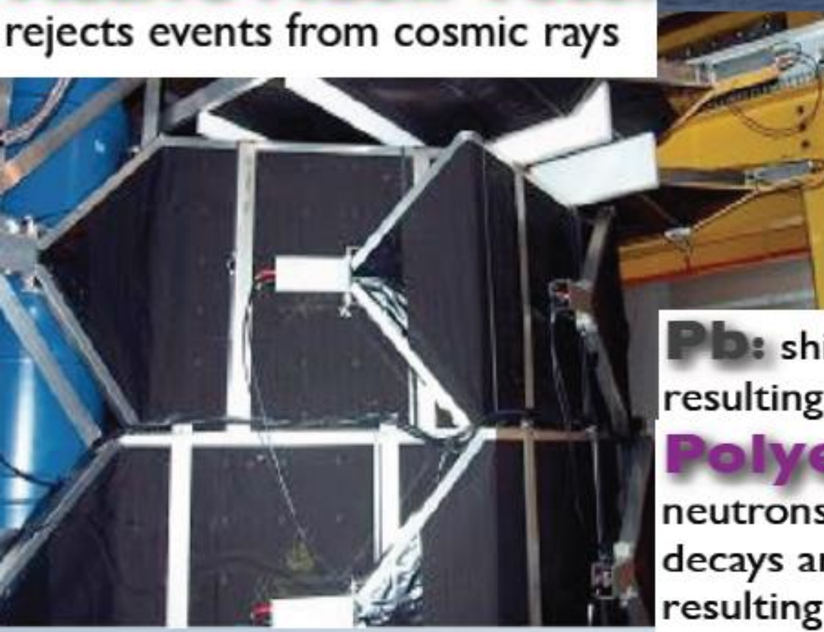
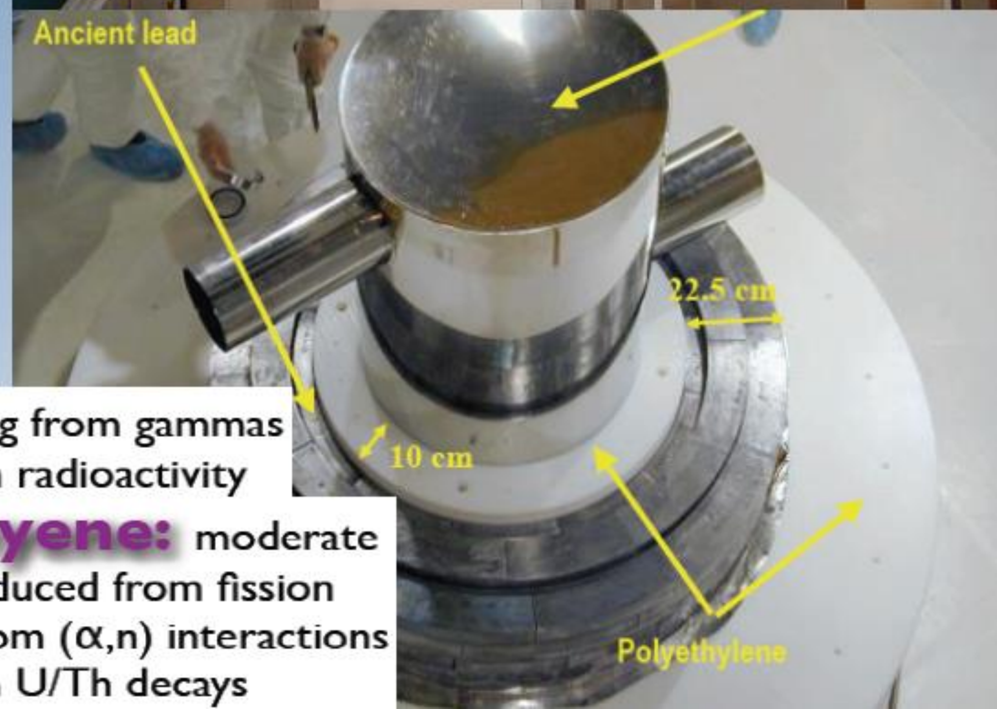
Backup slides

2100 mwe underground

Passive Shielding

Active Muon Veto:
rejects events from cosmic rays



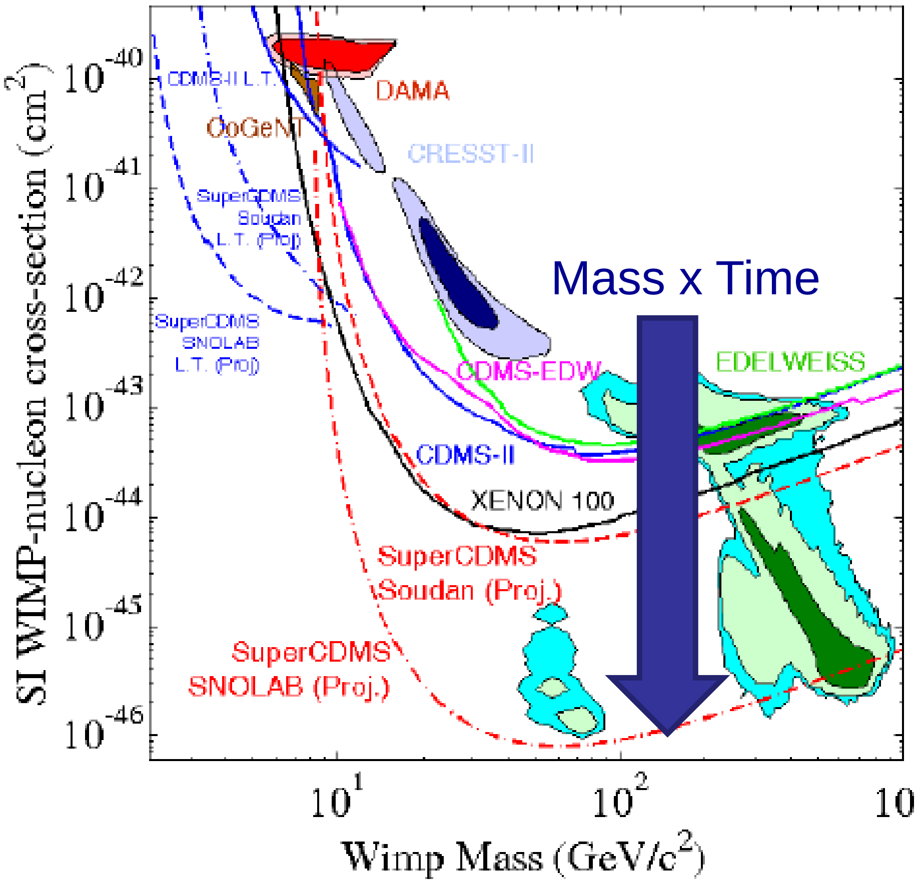


Pb: shielding from gammas resulting from radioactivity

Polyethyene: moderate neutrons produced from fission decays and from (α,n) interactions resulting from U/Th decays

Current and Projected Limits

- SuperCDMS Soudan will match current XENON 100 limit
- SuperCDMS Lite will produce world leading low-mass limits
- SuperCDMS SNOLAB to improve limit by two orders of magnitude



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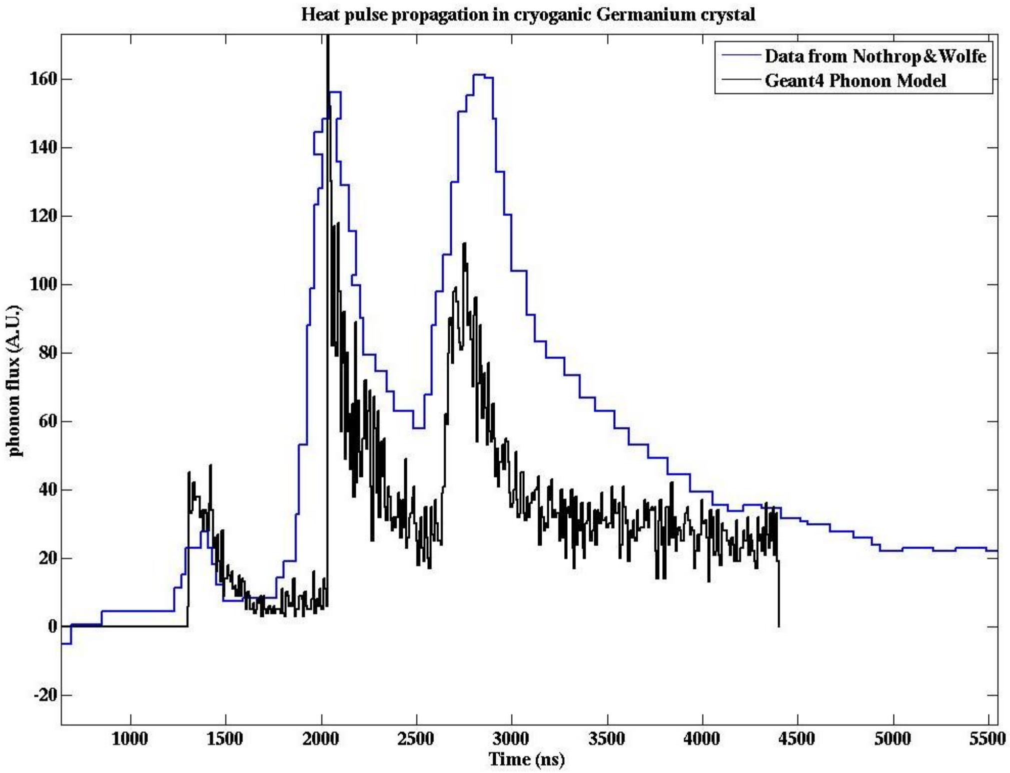
Validation of transport code



Phonon flux timing histograms, simulated (black) and observed by Nothrop&Wolfe (blue)

- Heat pulse propagation is a good test of phonon transport model
- Simulated heat pulse reproduces three peaks
- Simulation yields right branching ratios
- Discrepancies in onset time and Slow Transverse fall off are due to laser pulse shape and e^-/h^+ recombination

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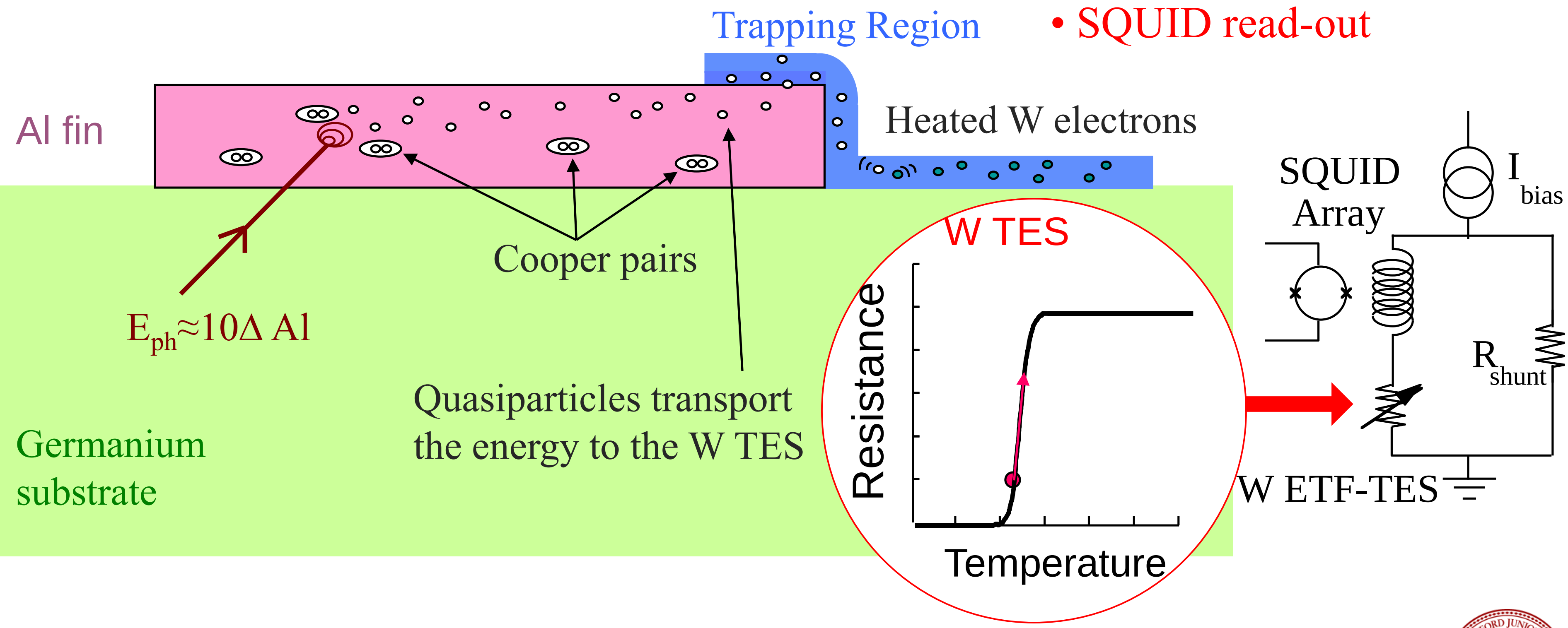
Phonon detection in CDMS

- Recoil event occurs in Germanium substrates, 76 mm diameter, 25 mm thick
- Aluminum fins 300 nm thick absorb phonons
- Fins connect to Tungsten transition edge sensors (W TESs)

- W $T_c \sim 80$ mK
- SQUID read-out



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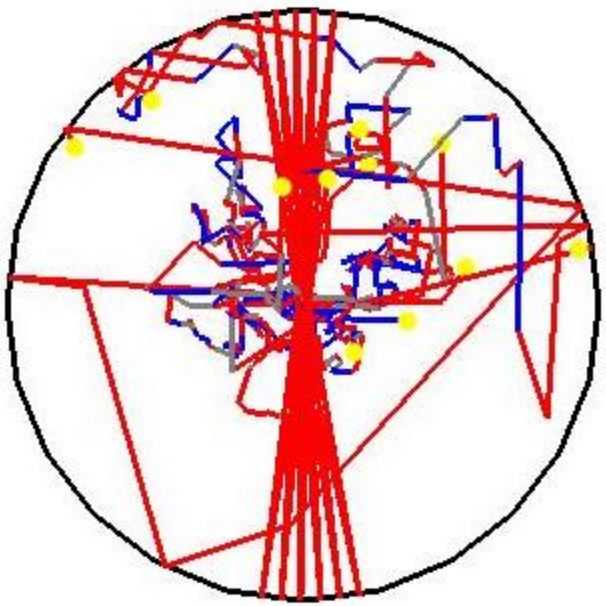
Quasi-diffuse Phonon Propagation



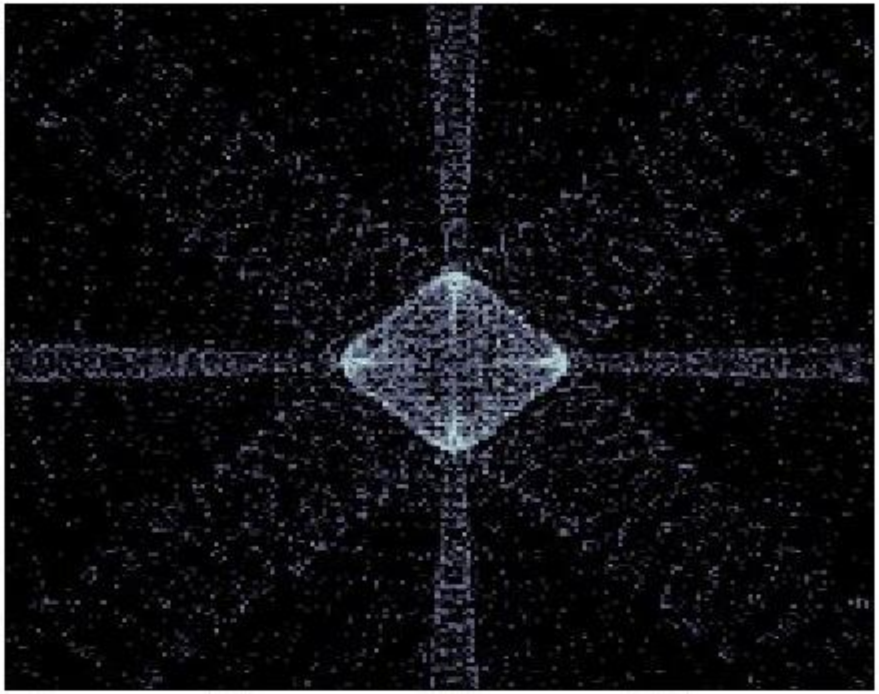
- Phonons of different energies have vastly different mean free paths

- Down conversion causes phonons to change from diffuse to ballistic propagation

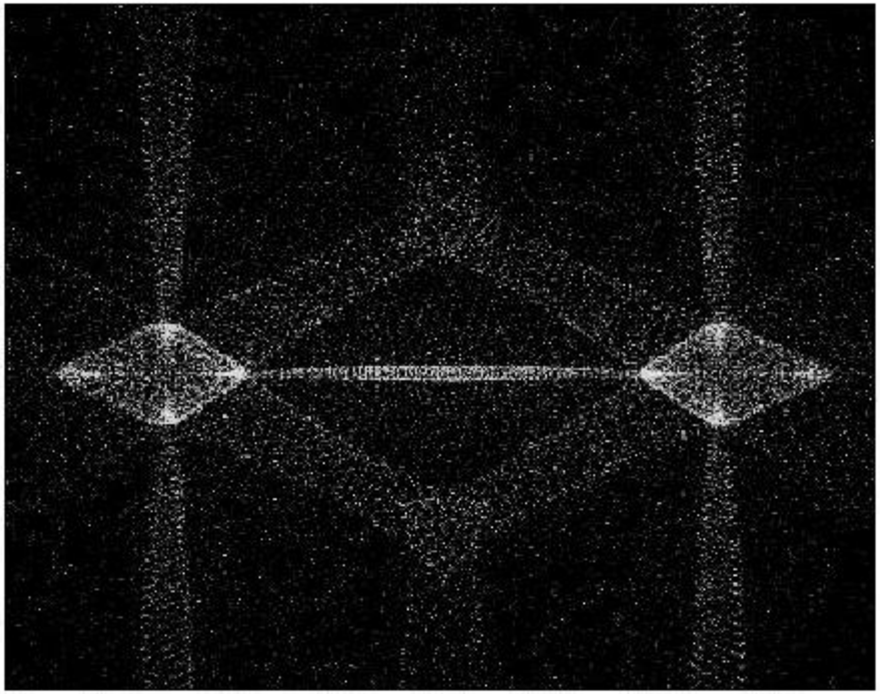
- This kind of quasi-diffuse propagation is difficult to model analytically

Phonon Focusing

Intensity patterns from a point source of phonons at the crystal center



Ge crystal in [001] orientation



Ge crystal in [111] orientation

Custom focusing maps

- Generate the Christoffel Tensor:

$$\begin{pmatrix} -v^2 + \frac{C_{11}}{\rho} & 0 & 0 \\ 0 & -v^2 + \frac{C_{44}}{\rho} & 0 \\ 0 & 0 & -v^2 + \frac{C_{44}}{\rho} \end{pmatrix}$$

- Find phase velocity:

```
Solve[{Det[Dij[{1, 0, 0}] - va] == 0, v ≠ 0}, v]
```

$$\left\{\left\{v \to -\frac{\sqrt{C_{11}}}{\sqrt{\rho}}\right\}, \left\{v \to \frac{\sqrt{C_{11}}}{\sqrt{\rho}}\right\}, \left\{v \to -\frac{\sqrt{C_{44}}}{\sqrt{\rho}}\right\}, \left\{v \to -\frac{\sqrt{C_{44}}}{\sqrt{\rho}}\right\}, \left\{v \to \frac{\sqrt{C_{44}}}{\sqrt{\rho}}\right\}, \left\{v \to \frac{\sqrt{C_{44}}}{\sqrt{\rho}}\right\}\right\}$$

- Build group velocity vectors:

```
Needs["NumericalCalculus`"]
vgroup[index_, {x_, y_, z_}] :=
 {ND[v[index, {X, y, z}], X, x],
  ND[v[index, {x, Y, z}], Y, y],
  ND[v[index, {x, y, Z}], Z, z]}
```

Motivation: SuperCDMS Detector Monte Carlo

- SuperCDMS background rejection: energy partitioning between phonon and charge channels
- Requires excellent understanding of the phonon signal resulting from real background distributions → Geant4