Phonon Transport on Geant4

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Phonon transport on Geant4: Motivation

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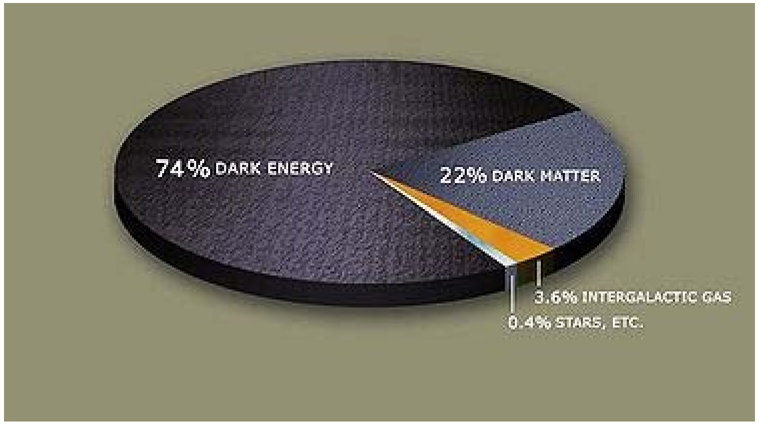
- According to cosmology, 22% of the universe is composed of dark matter
Image taken from en.wikipedia.org



- The nature of dark matter remains a mystery

- The Cryogenic Dark Matter Search (CDMS) experiment attempts the direct detection of dark matter

- The CDMS detection strategy requires a detailed understanding of phonon transport in semiconductor crystals.
Image taken from cdms.berkeley.edu

Project Overview

Project Goals

1) To implement phonon transport in Geant4 to support the CDMS experiment.
    - o Implementation of crystal lattices, phonons as G4Particle and phonon processes at cryogenic temperatures

2) To achieve a well integrated and general implementation of phonon transport processes that can be shared with the community

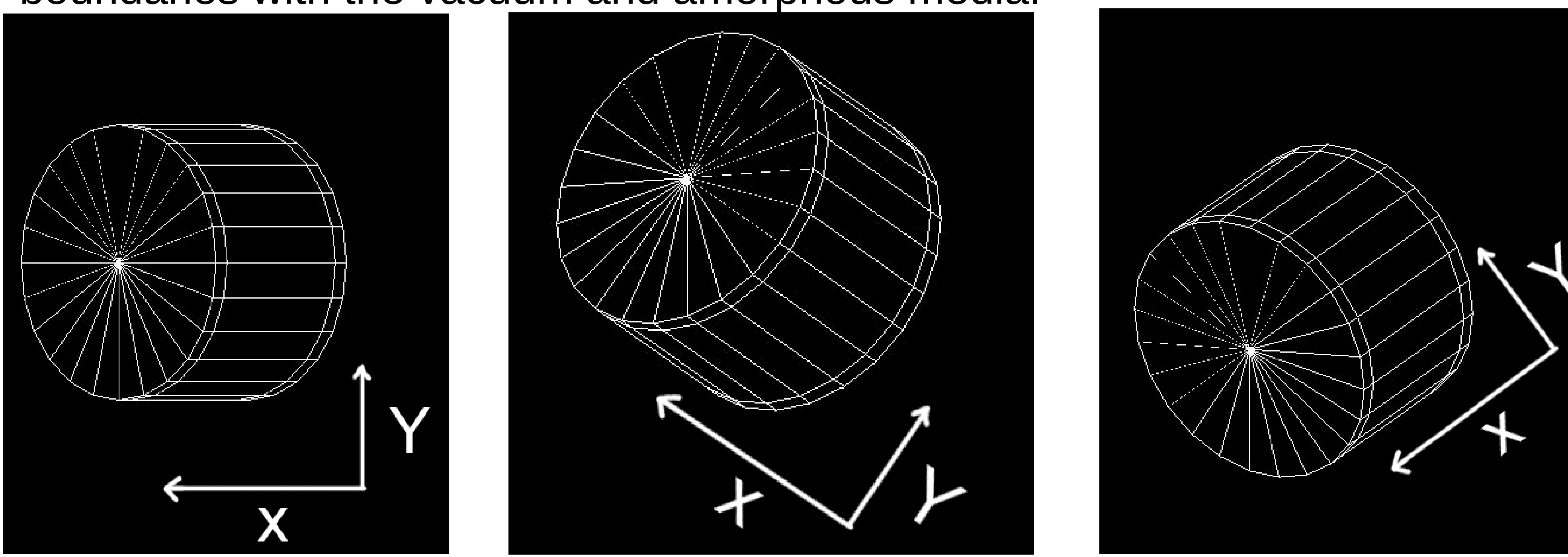
The underground site of superCDMS at SNOLAB, Sudbury. *Image taken from bbc.co.uk*

Seamless integration with Geant4

Our implementation aims to allow users to treat phonons just like any other particle.

Lattices are created at during detector construction and associated with the relevant physical volume.

Once a lattice is created, the simulation code takes care of all re-orientations and coordinate transforms. The code automatically handles boundaries with the vacuum and amorphous media.



Technical Challenges

Two major challenges had to be overcome in order to allow phonon implementation in Geant4:

1) In Geant4, zero rest mass particles move at the speed of light. **Phonons have zero rest mass but move much more slowly than the speed of light** (a few thousand m/s).

2) Geant4 materials are isotropic and independent of physical volume orientation. **The concept of an anisotropic crystal is pivotal to phonon transport in semiconductors**.

Both of these problems have been overcome, and anisotropic slow zero rest mass phonon transport has been implemented in a phonon transport test code.

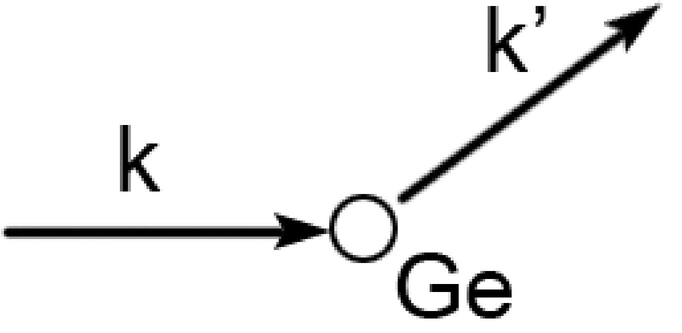
Phonon Processes

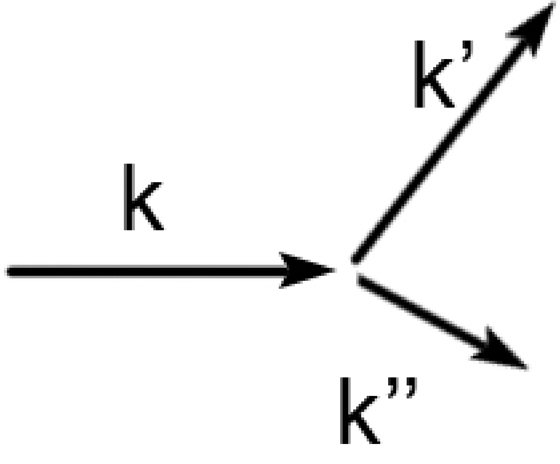
Relevant phonon processes

The CDMS Ge crystals are operated at **cryogenic temperatures of order 40 mK**.

To first order, the transportation processes relevant to phonons in the CDMS crystals are:

1) Isotope scattering and mode mixing





2) Anharmonic down conversion

Phonon focusing

Isotope scattering is **not isotropic in velocity space**, but in k-space. A scattering event randomizes a phonon’s wave vector.

The anisotropic elasticity of crystals leads to phonon transport being **focused along preferred directions in the crystal**. The resulting intensity patterns are called *caustics*.

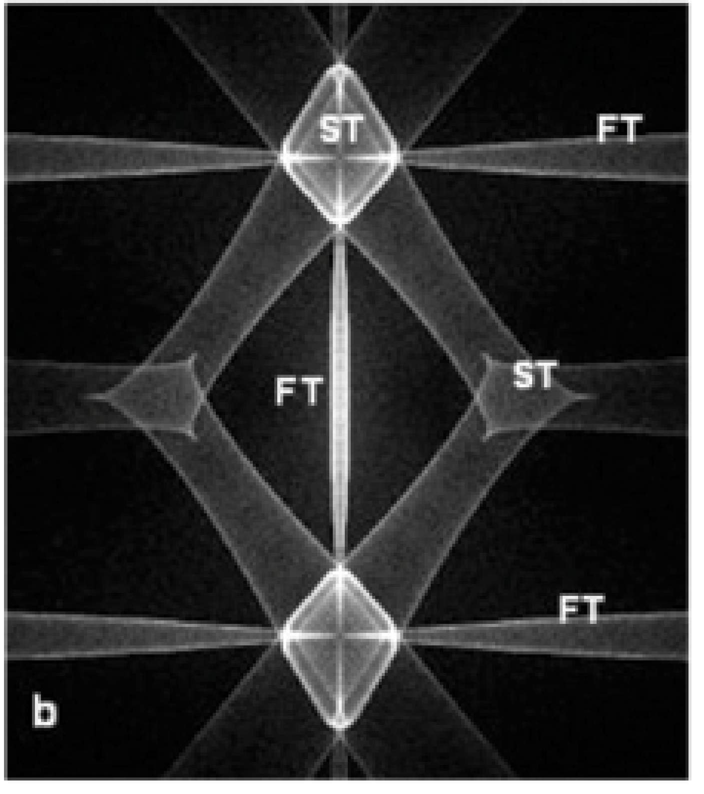


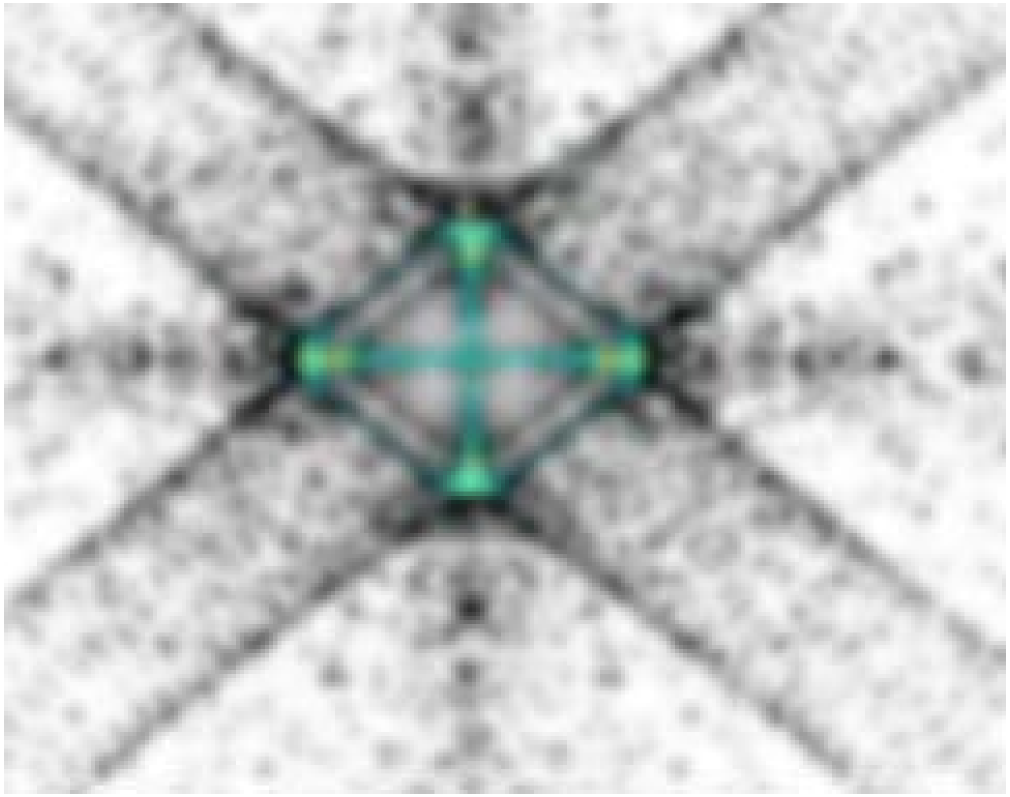
Image taken from Jakata & Every[1]

[1] Jakata & Every , S.Afr.J.Sci 104 (2008)

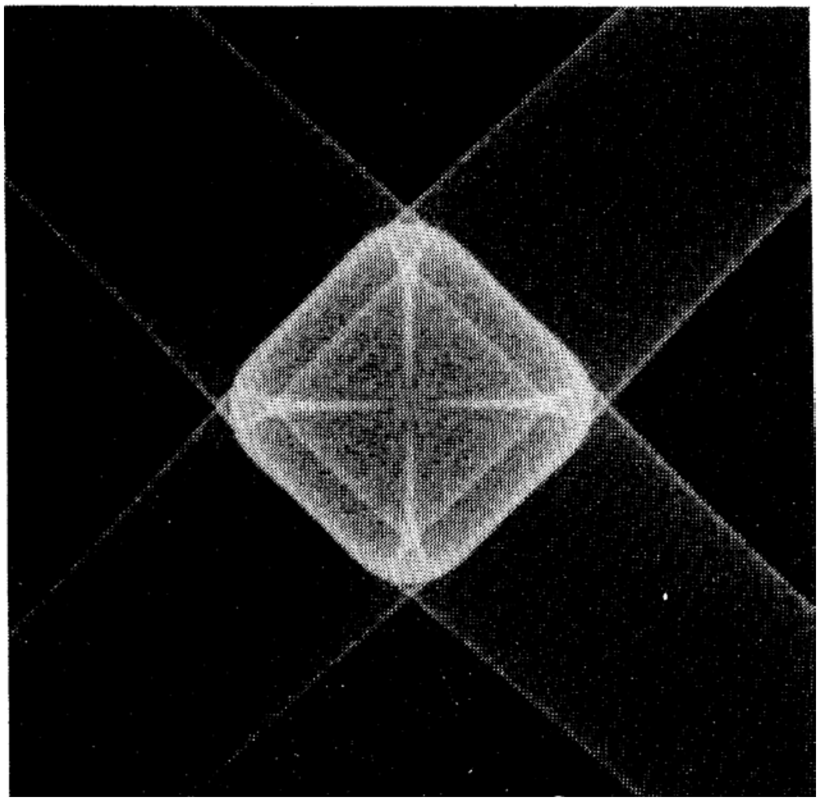
Simulation Outputs

Validating phonon focusing

Simulated phonon focusing patterns for Slow Transverse (ST) polarized phonons scattering at the center of a Ge crystal are a good qualitative match for experimental results.



Simulated Ge caustic



Experimentally recorded Ge caustic[2]

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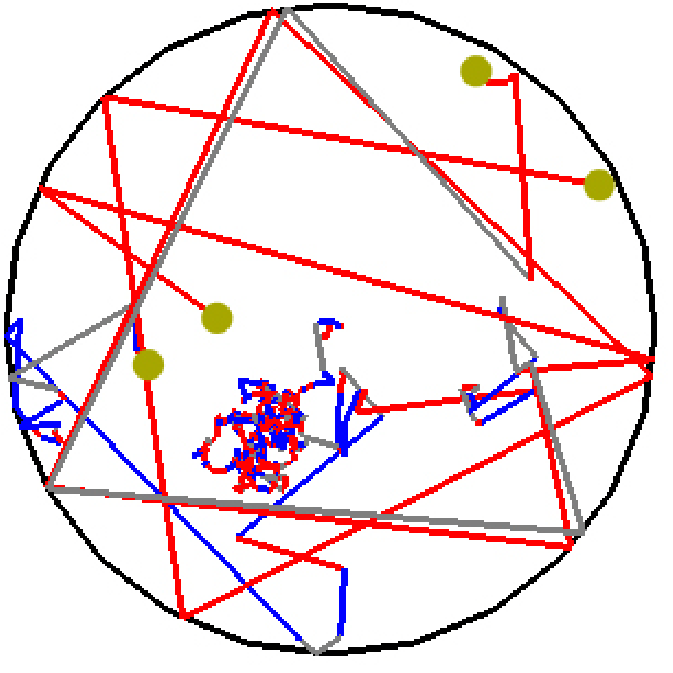
[2] Hurley and Wolfe, *Phys. Rev. B* **32** (1985)

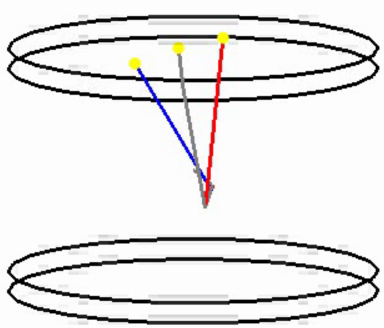
Quasi-diffuse propagation

Scattering and down conversion mean free paths scale as E_{ph}^{-4} and E_{ph}^{-5} respectively

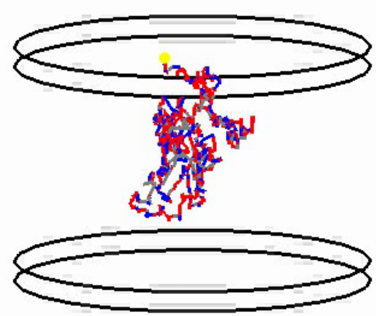
The resulting propagation behavior is known as quasi-diffuse propagation. Quasi-diffuse propagation is difficult to analyze analytically.



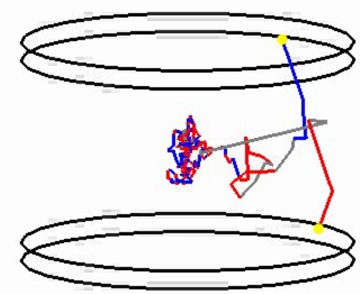
Simulated transport processes



Down conversion



Scattering/
polarization change



Down conversion +
scattering / pol. change

Phonon transport in Geant4: Demonstration

Summary

• Implemented phonons as Geant4 particles

• Implemented crystal lattices as part of physical volumes

• Phonon focusing in crystal lattices gives good match to experiments

• Implemented all phonon-only processes relevant to CDMS:
  - Isotope scattering
  - Mode mixing
  - Down conversion
  - Specular reflection

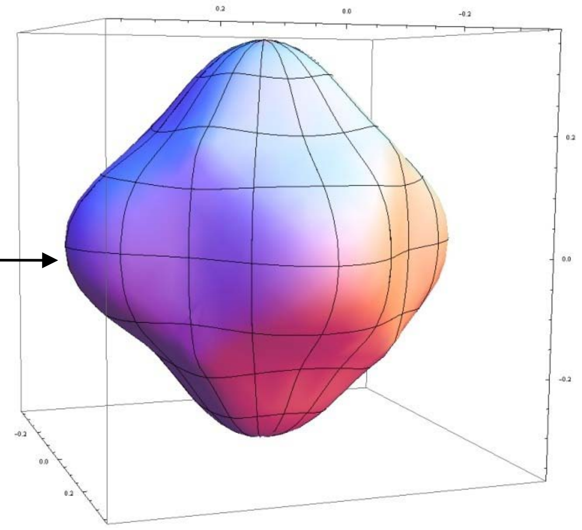
• **Have a complete, self consistent framework for cryogenic phonon propagation in semi conductor crystals**

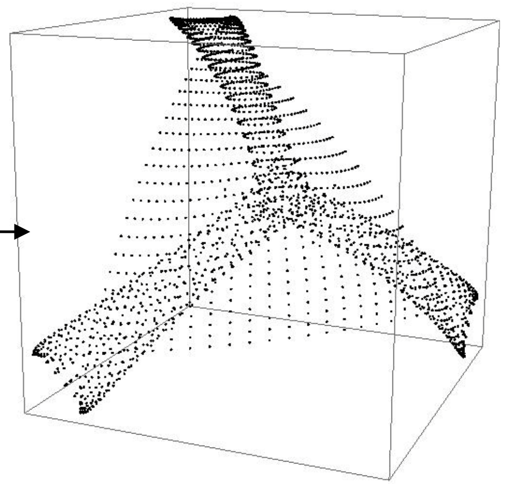
• Next steps are to include phonon emission by electrons and phonon-photon conversion at free boundaries

Phonon focusing: Mathematical model

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

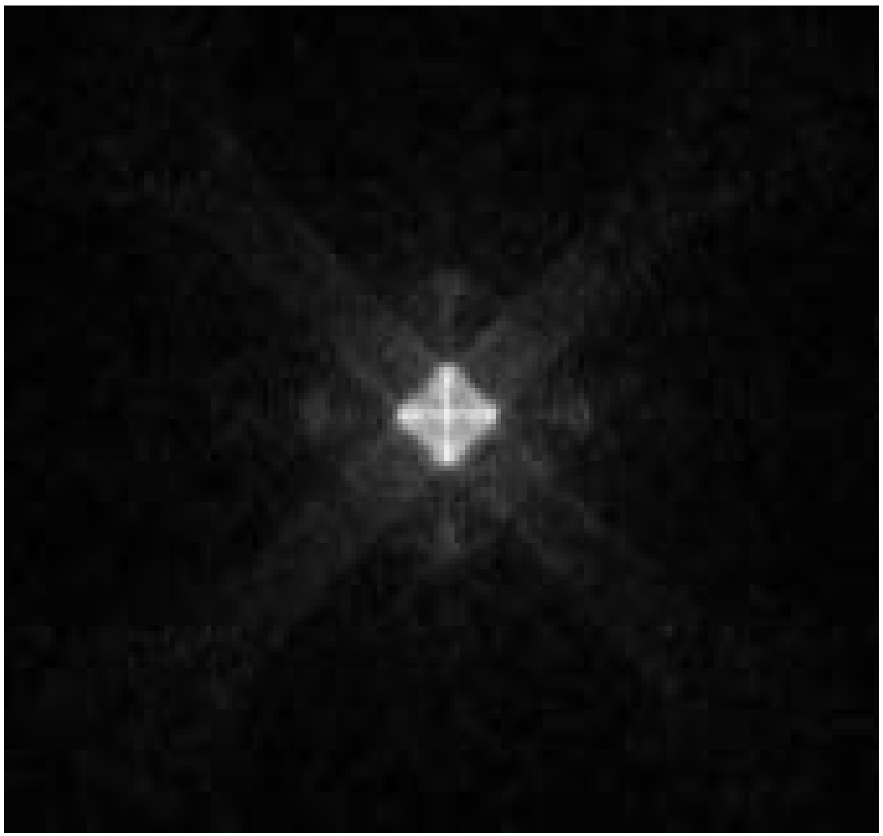
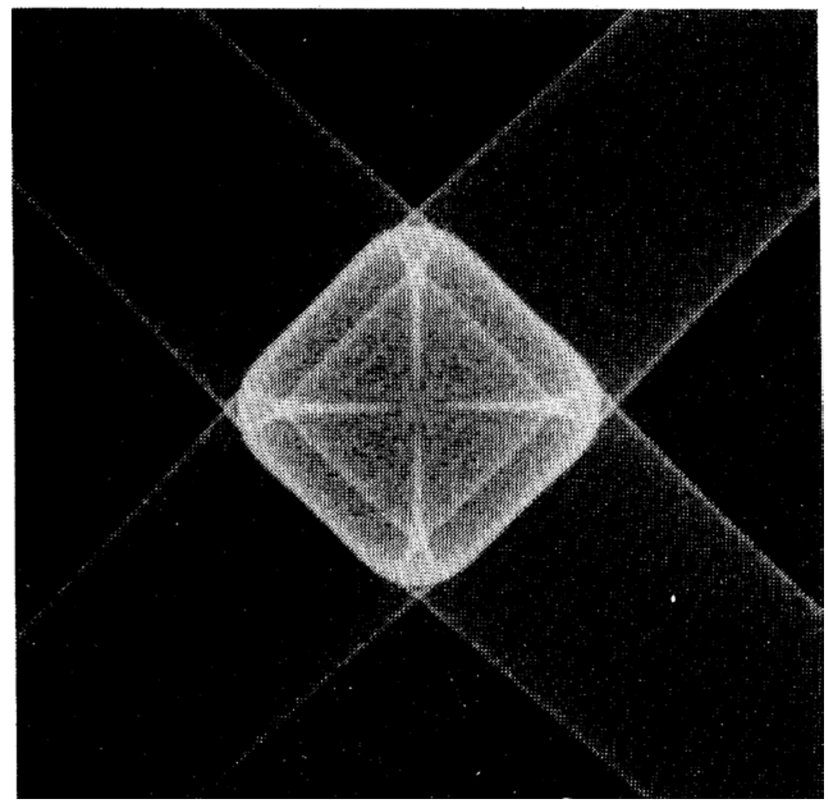
n=wave vector direction
v=phase velocity ~ frequency ω
e=polarization vector
ρ=local mass density





Solve for the eigen-vectors of the 3D wave equation

Find the gradient vector at each point to determine the corresponding V_g.

Phonon transport on Geant4: Status summary

- **Phonons have been implemented as Geant4 particles**

- **Crystal lattices have been implemented as new C++ class**
    - Lattice class handles crystal orientations and rotations of physical volume

- **Phonon group velocity as a function of wave vector**

- **Isotope scattering implemented as G4VDiscreteProcess**
    - Computes mean free path
    - Generates scattering wave vector
    - Computes focused group velocity
    - Handles mode mixing

- **Anharmonic down conversion implemented as G4VDiscreteProcess**
    - Computes mean free path
    - Generates correct energy partitioning
    - Conserves pseudo-momentum

- **Phonon reflections implemented as G4VDiscrete Process**
    - Assumed specular