G4CMP: New Physics for Superconducting Devices

Noah Kurinsky
Staff Scientist, SLAC
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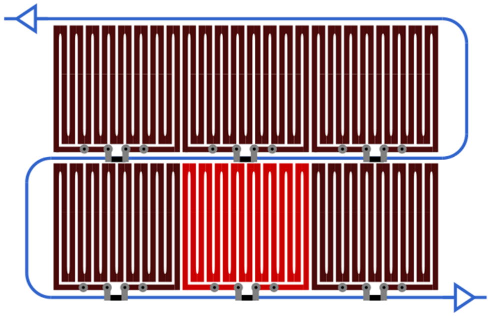
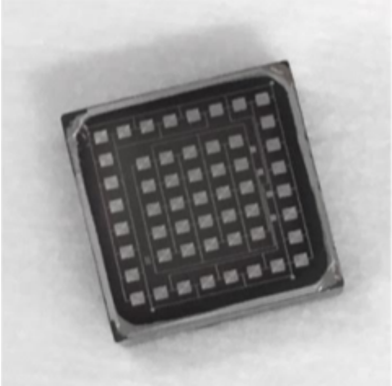
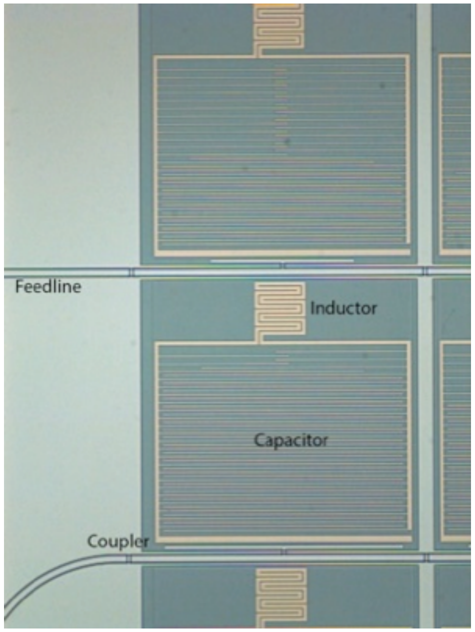
BOLD PEOPLE. VISIONARY SCIENCE. REAL IMPACT.

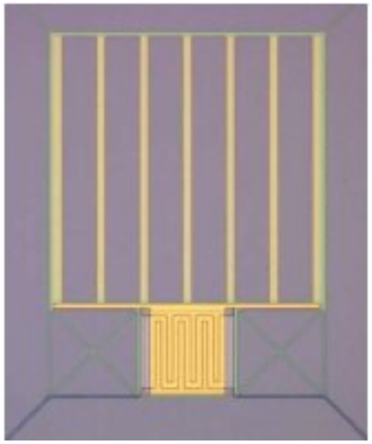
Outline

- Setting G4CMP Context
  - Overview of process additions
- Adding materials
  - Charge transport
  - Scintillation
  - Phonon transport
- Extending functionality
  - Sub-gap phonon losses
  - Modeling QP dynamics
- Prompts for discussion









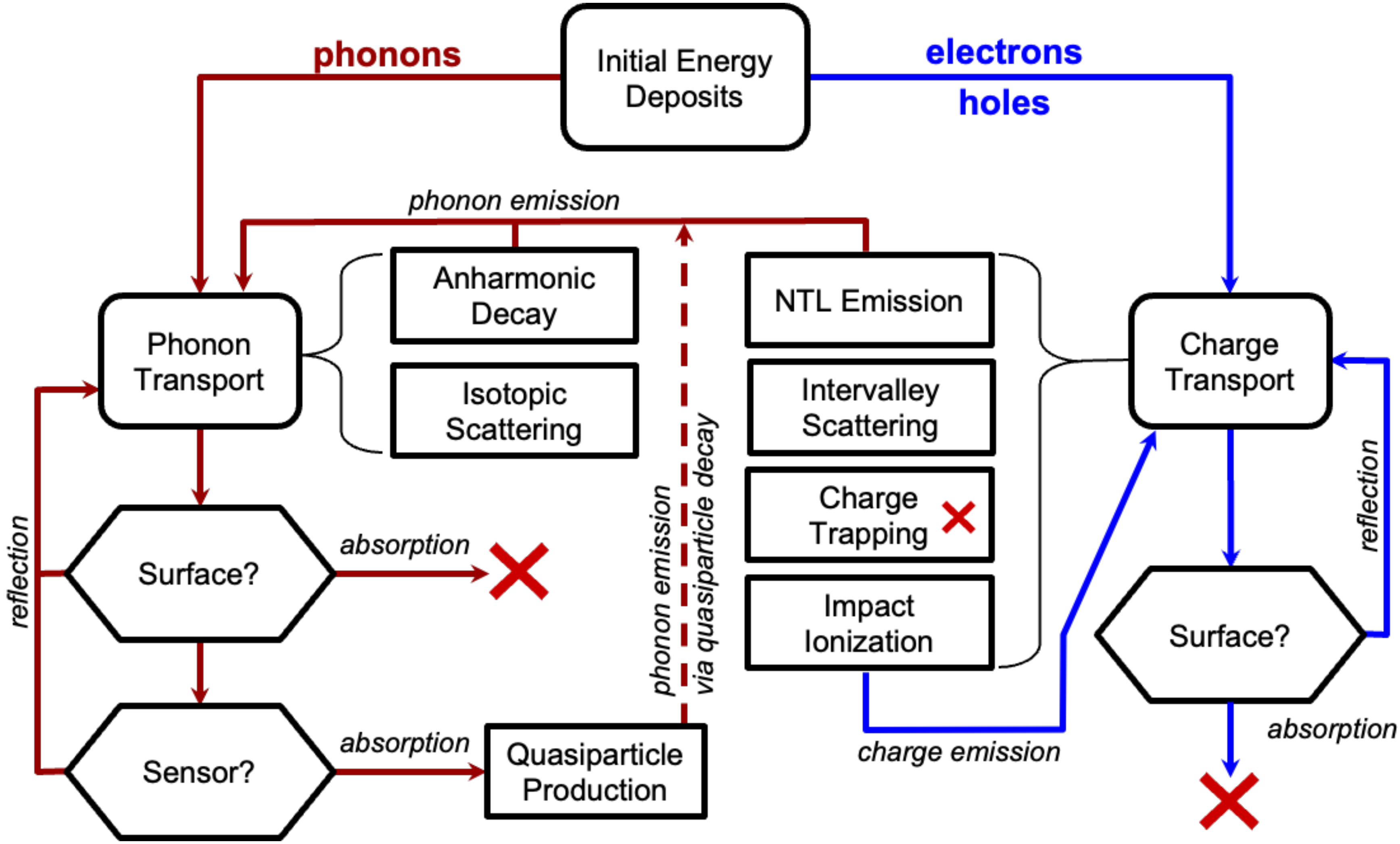
G4CMP: Remembering our History

- Keep in mind that G4CMP was primarily developed to understand radiation detectors at the keV scale - all of the new processes that are being developed are meant to address side-cases that were not considered
    - G4CMP couldn't be run without a field for charge collection
    - Normal metals aren't implemented explicitly
    - We only have Si and Ge - and we only considered substrates with indirect gaps (no scintillation)
    - Only cubic crystal lattices are considered

- In extending our modeling to a new regime (high-voltage operation for SuperCDMS), we started to revisit some of the basic physics and already improved some processes
    - Better intervalley scattering models at high energy
    - Including effects of charge trapping

- For generic superconducting applications, we need to broaden our horizons
    - Substrates vary more broadly - sapphire is a widely used substrate
    - Sensor designs change faster and are less spatially uniform
    - Multiple types of absorbers/metalizations are used, compared to only Al
    - Sensors care about different dynamic effects
    - Substrate effects are subdominant to effects of substrate interactions on surface layers - the physics in the surface layers now becomes equally important

What’s Missing from These Blocks?



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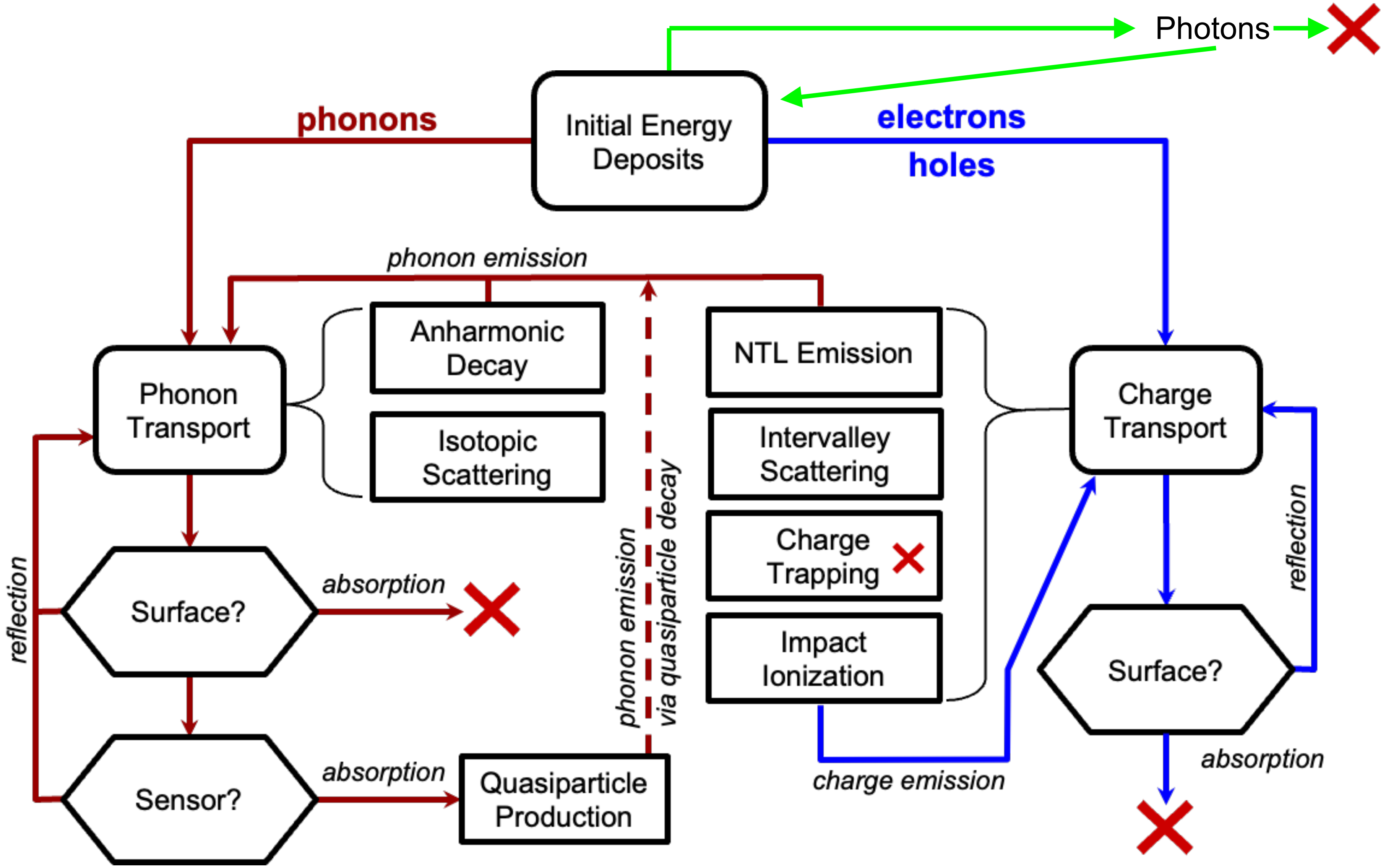

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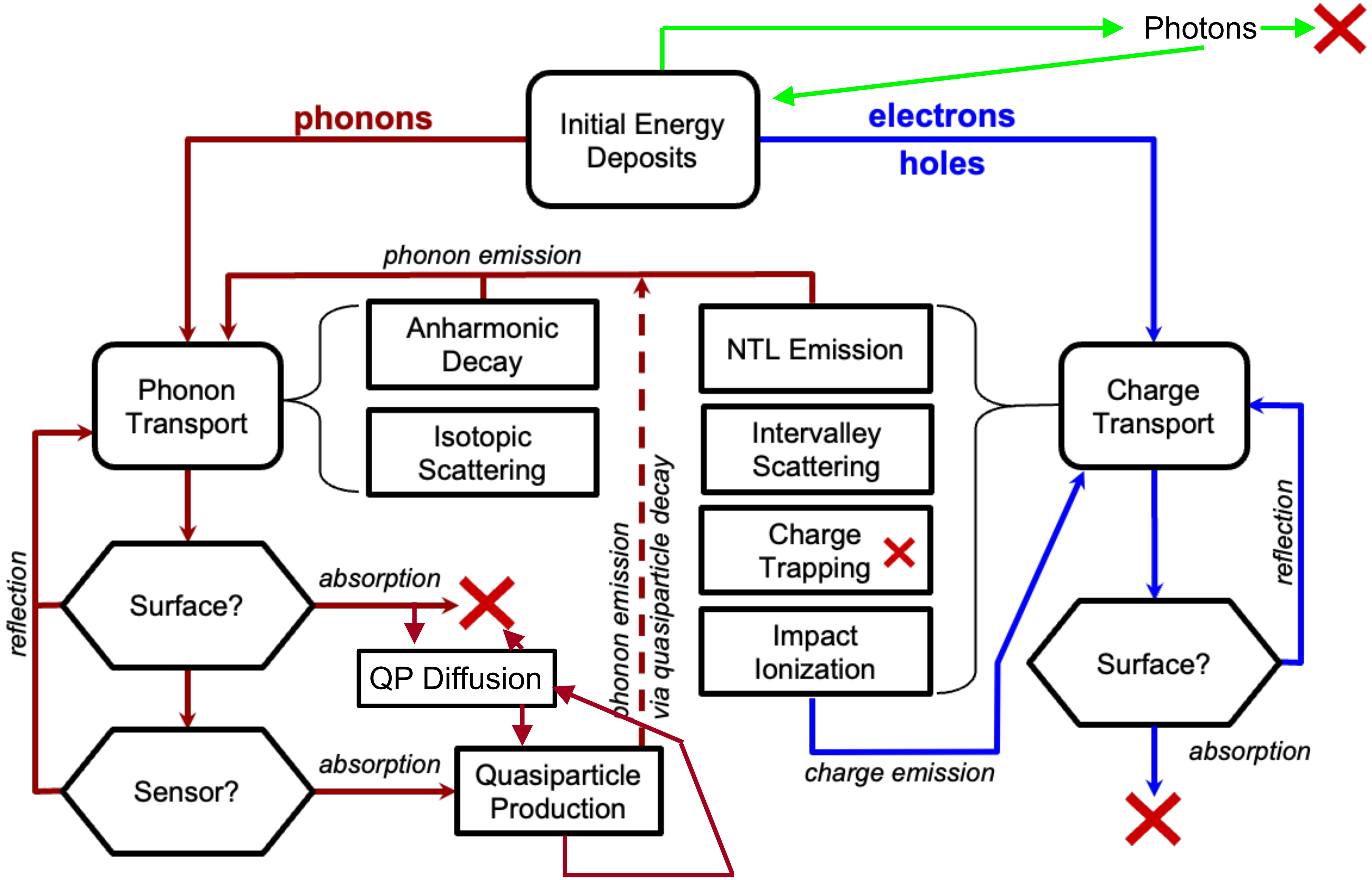

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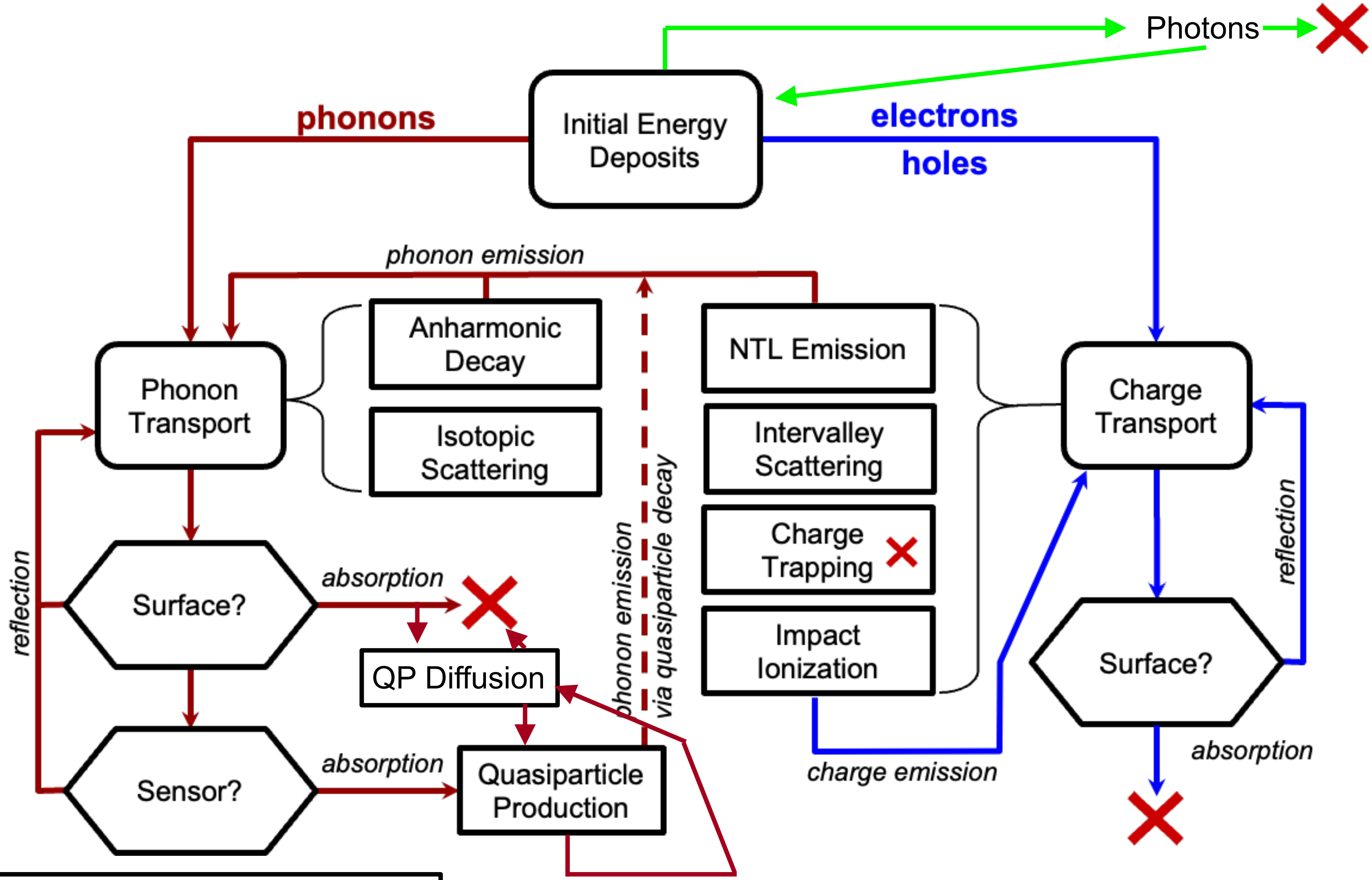

Angle, Material, Mode Dependence

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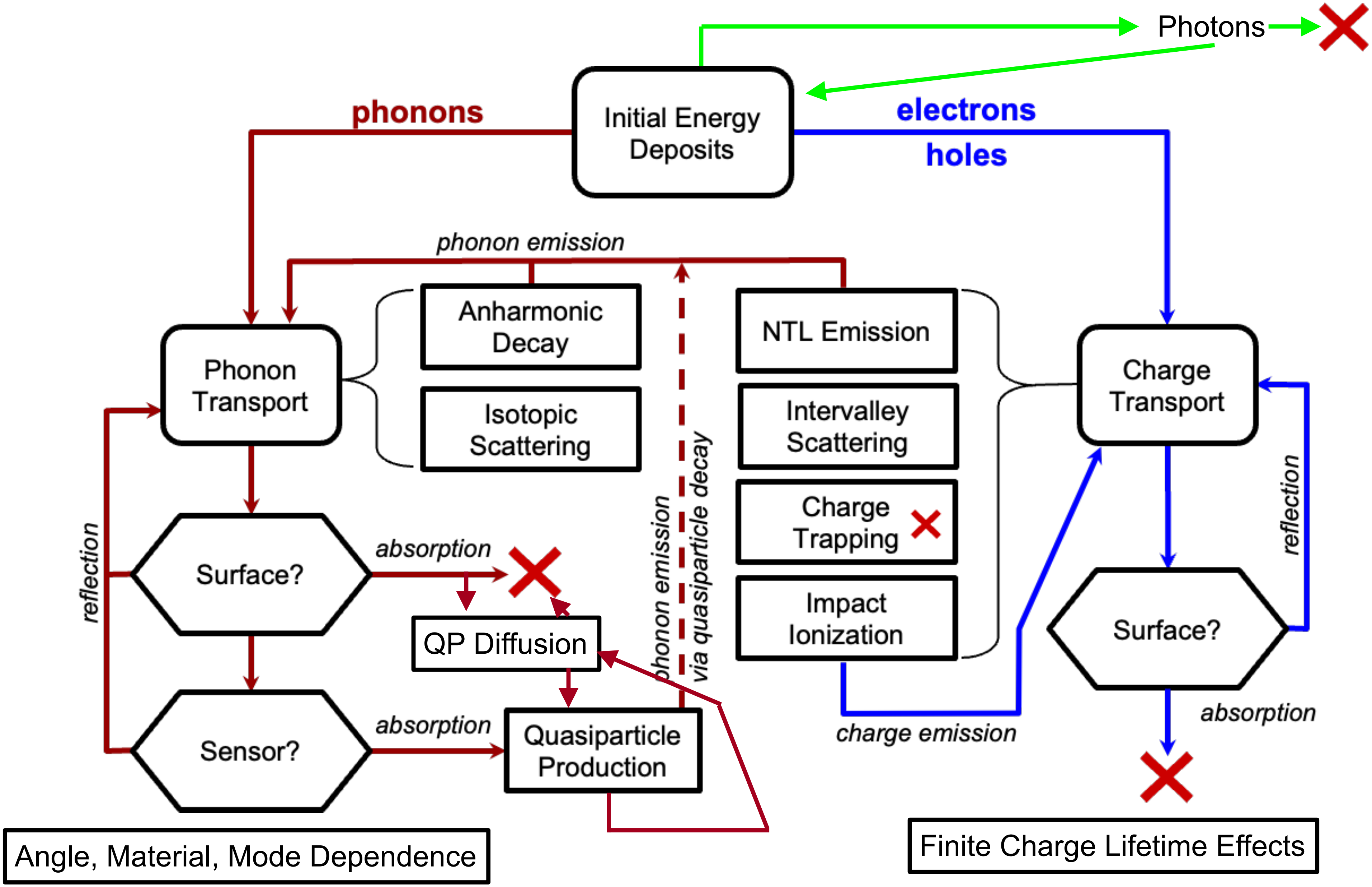
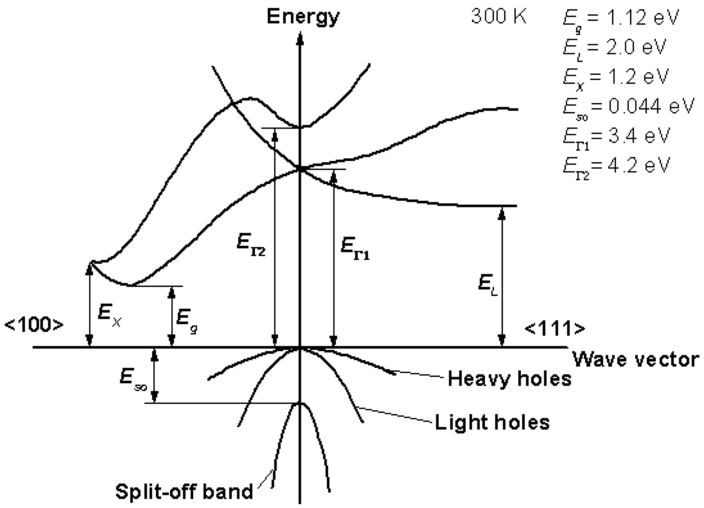


Angle, Material, Mode Dependence

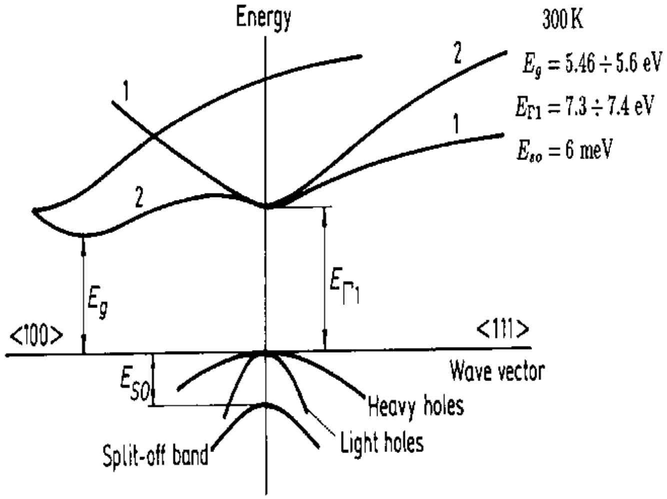
Finite Charge Lifetime Effects

G4CMP Materials

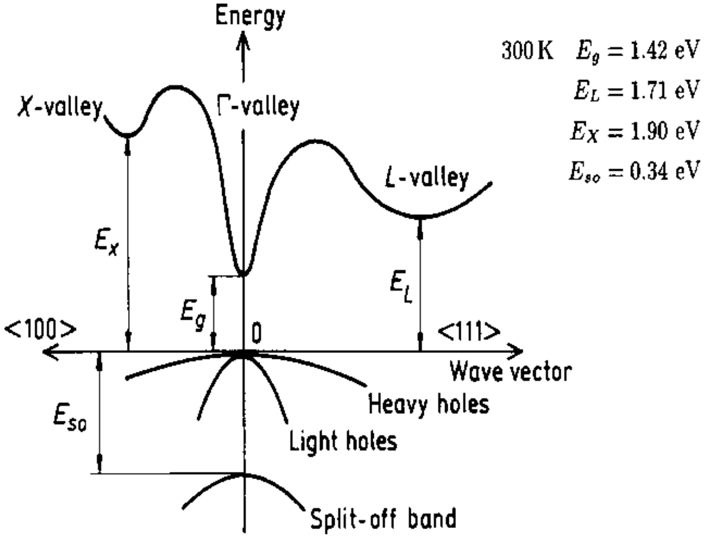
Si



Diamond



GaAs



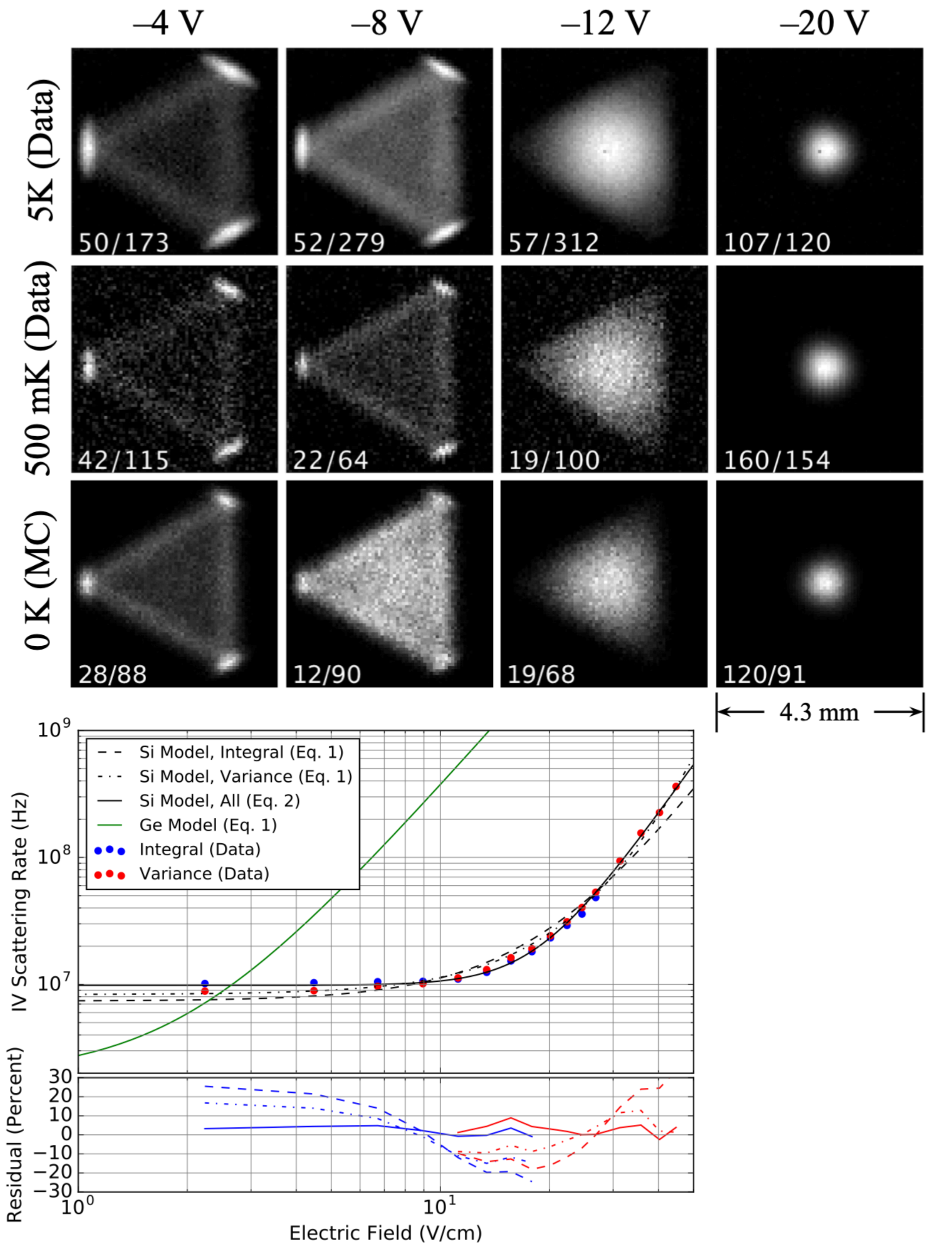
- How easy it is to adapt new materials depends on how well our models adapt to new structures?
  - Well developed and calibrated: Ge, Si
  - Some work to add charge transport: Diamond, SiC - similar in behavior to Ge, Is
  - Scintillators don’t fit the model of long-lived charge decaying only into phonons

- Work done to add phonon transport: Sapphire, LiF, GaAs, more? (see I. Alatorre’s talk)
  - Phonon structure was always more complex, so a full treatment was developed

G4CMP Material Validation: Charge Transport

- Charge transport was hard to tune in order to get mm-scale patterns correct
    - Ge and Si substrates specifically fabricated with a laser scanning system to produce calibration data
    - This was used to inform models of intervalley scattering

- In principle, this would need to be repeated for other indirect-gap materials, though we were able to fit to a model informed by optical phonon emission



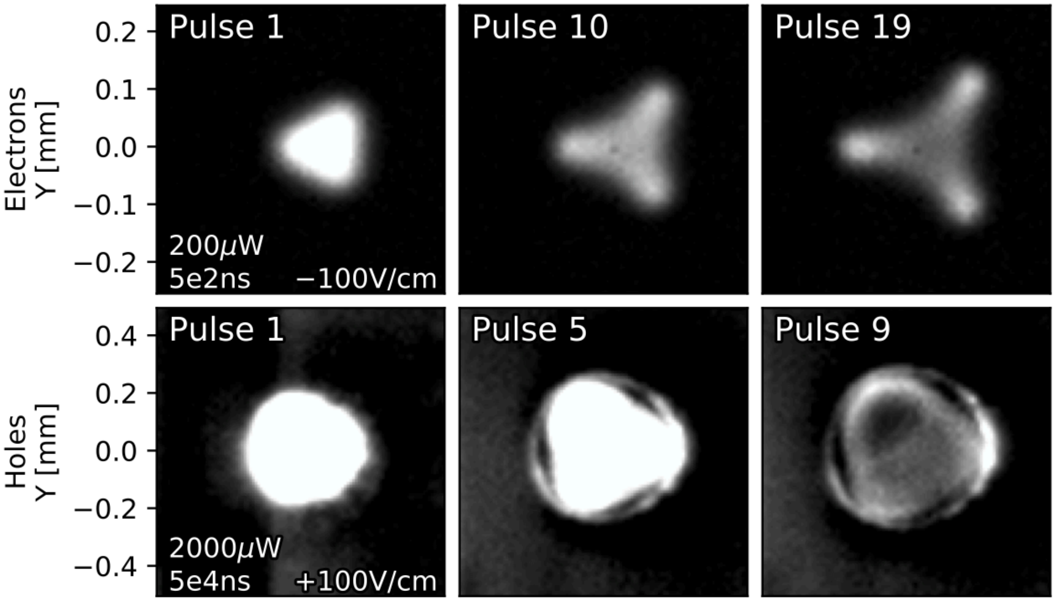
G4CMP Material Validation: Charge Transport

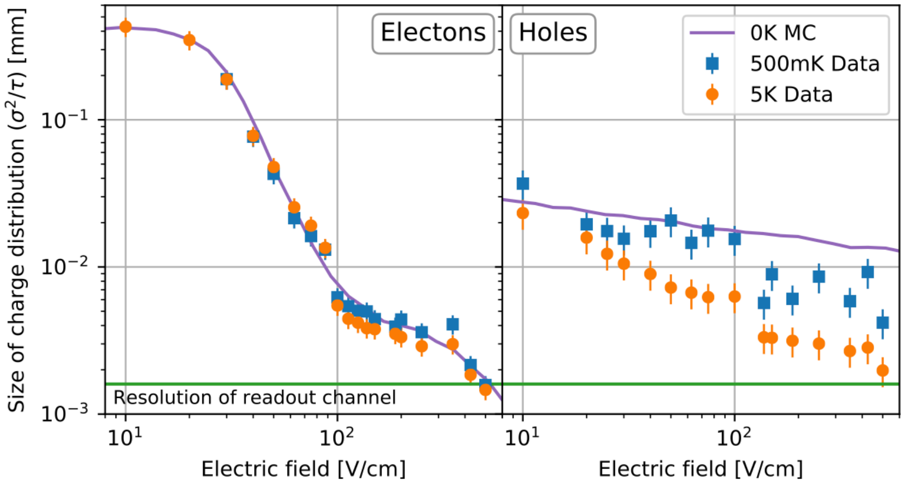
- G4CMP does not simulate space charge effects, and these can become appreciable for large numbers of events or small charge patterns

- This data was taken at high voltage (this is what one might expect for hole transport or more isotropic crystals)

- Keep in mind that, if you see time-dependence in charge accumulation, this is an effect that will be need to be added by hand
    - What's more - G4CMP doesn't deal with charge recombination explicitly. Think about space charge when running high-intensity experiments and consider ways of neutralizing your crystal

arxiv:1910.02169 (Si)





Charge Transport Open Issues and Upgrades

- Number, direction, and effective mass of valleys in new materials is not hard to implement if measured
  - Number is only relevant for long-lived charge states in indirect-gap materials - most of the new materials can be modeled as isotropic, which would also imply short charge lifetime

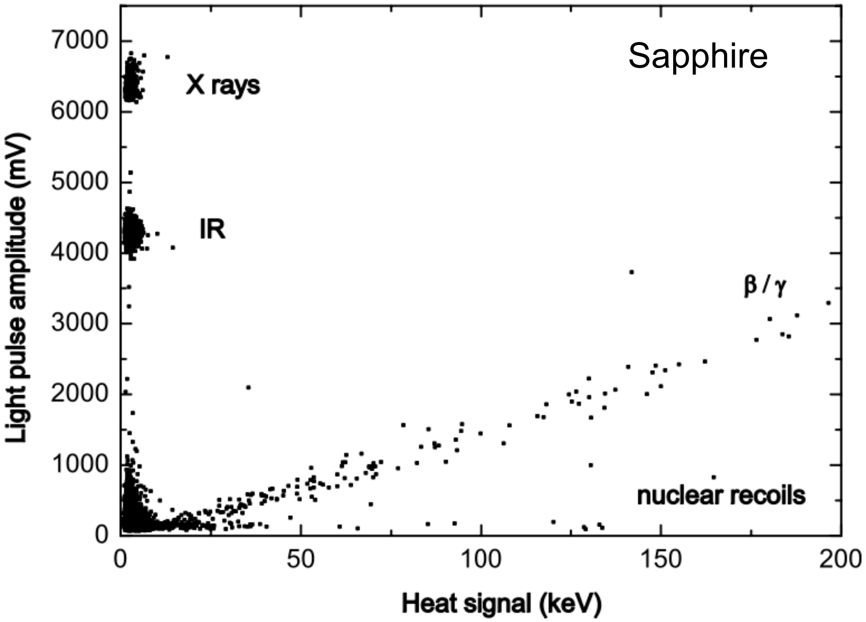
- Inter-valley scattering is an open problem for long-lived charge propagation - the rate is defined by optical phonon emission, which we don’t currently implement
  - This means high-voltage electron propagation needs a similar calibration campaign or the spatial distribution won’t make much sense

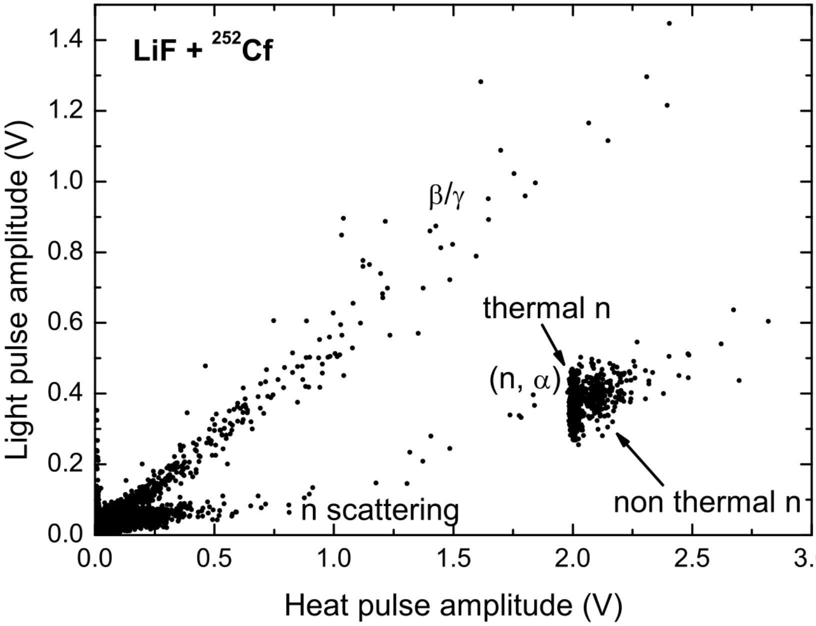
- Short charge lifetime is not something that was initially considered
  - For 0V simulations, we implemented finite charge lifetime as a trapping mean free path. It’s phenomenological and doesn’t full

Handling Scintillation: Re-emission in GEANT4

- An open problem that G4CMP doesn't directly deal with is energy release from killed charge tracks
  - This is an issue in Si/Ge for final recombination, which is only relevant for incomplete charge collection
  - For direct-gap substrates this is the leading-order loss for electronic recoils and likely the predominant source of spatial cross-talk due to radiation

- This is not really a G4CMP problem to solve - photons are a GEANT object - but we've never explicitly treated scintillation
  - Should this be done at the initial event stage?
  - How do we handle trapping/recombination if we do want to produce drift charges?





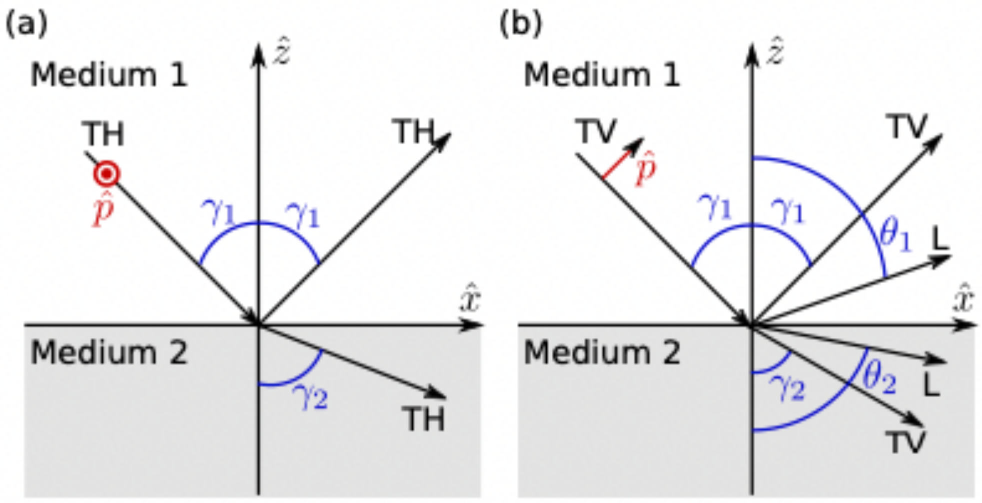
Phonon Physics: What Are We Missing?

- What don't we implement?
  - Optical phonons don't exist in G4CMP - that is likely only a problem for inter-valley scattering but does limit accuracy of high-energy phonon transport
  - We don't track phonon polarization, though handles exist for that - this could be done if important

- What should be improved?
  - Propagation within crystals is robust, we just need to document procedures to extend to new materials (see e.g. I. Hernandez talk)
  - Reflection at interfaces is vastly over-simplified and needs to be improved
  - Normal metals don't officially exist, but would be easy to implement
  - Phonon propagation within surface layers can also be implemented - that's not fundamentally different than in crystals!

Phonon Reflection and Transmission: Full Model

- Kaplan model of phonon reflection is very reminiscent of snell’s law - the relevant parameters are differences in media density and phonon density of states
- This reflection is angle dependent and mode dependent, and will vary for any given crystal/film combination
- This is fairly easily tabulated given sound speeds and relative phonon DOS



Material	Al	Nb
τ_0^{ph} [ps]	242	4.2
c_s [μm ns^{-1}]	3.58	2.44
λ_{ph} [nm]	860	10
$2\Delta(\mu\text{eV})$	360	3000
p_{in} [Si]	0.795	0.745
p_{out} [Si]	0.29	0.13
f_{cov}	1%	10%

Table 1: Example parameters for Al and Nb films for a test device.

Limitations of Current Implementation

- Reflection at interfaces (where there is a chance of transmission) is set by a fixed, angle and mode averaged probability
  - It will technically need to be re-tuned for all substrate/film pairs, though for a given substrate it won't vary substantially
- There is no explicit treatment of internal reflection within films
  - Phonons are re-emitted from KaplanQP depending on a random emission angle, but this is a rough treatment
- We have historically validated this reflection coefficient using phonon collection time - that's only possible in low-coverage devices, and degenerate with other loss/absorption mechanisms

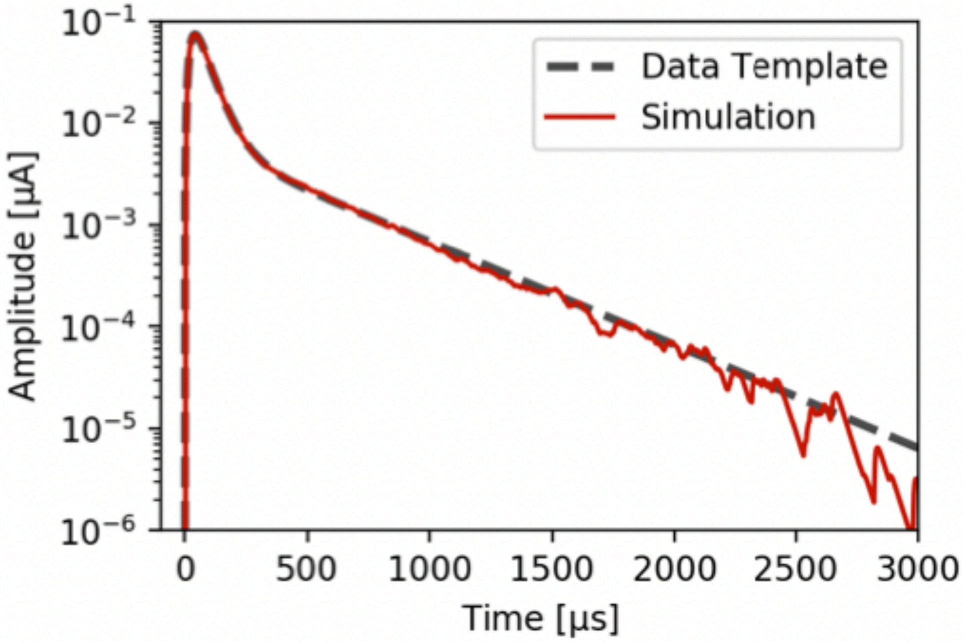


Figure 9: Parameter-optimized phonon pulse response simulated for an HVeV device using G4CMP and the SuperCDMS Detector Monte Carlo (red solid), compared to the pulse template constructed from HVeV laser calibration data (black dashed).

Multiple Surface Volumes are Possible

- G4CMP, like GEANT, can have many types of materials all in the same simulation - there is no limitation to have a single film type or crystal type
- For improved utility, we need to include a demo that shows how to implement multiple film types including material and thickness variation - Ryan will cover some of this in his tutorial
- To accurately include boundary effects in a directional manner, we need to take some features from GEANT4 optics, which would imply implementing boundaries inside the film volume as well as inside the crystal volume
  - This also means treating the film as a true volume G4CMP - more on this in a minute

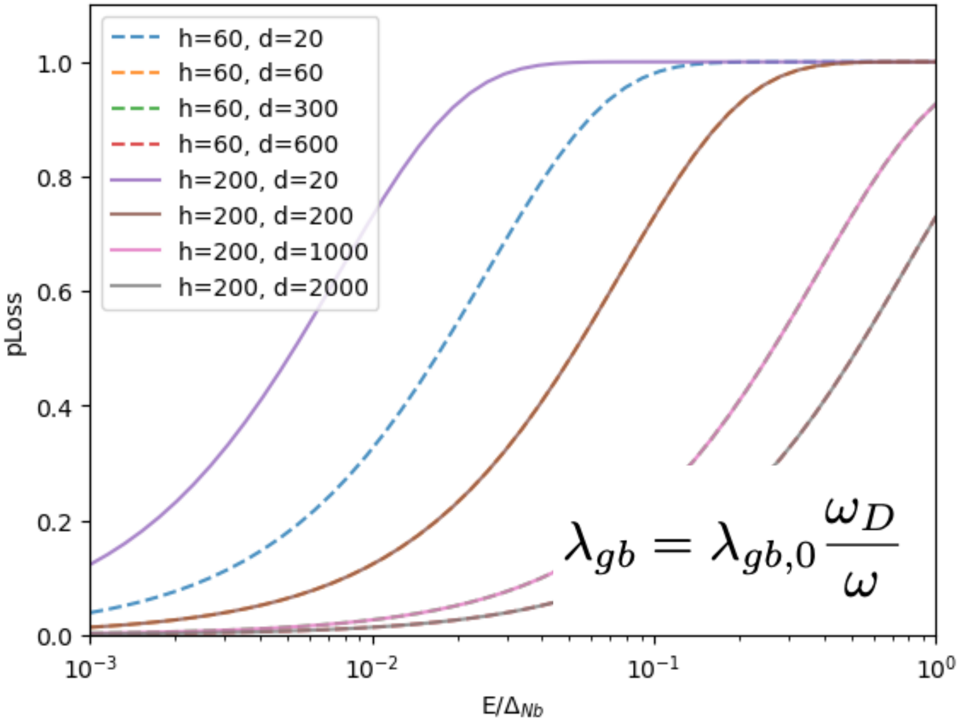
```
//Germanium lattice information
//

// G4LatticeManager gives physics processes access to lattices by volume
G4LatticeManager* LM = G4LatticeManager::GetLatticeManager();
G4LatticeLogical* GeLogical = LM->LoadLattice(fGermanium, "Ge");

// G4LatticePhysical assigns G4LatticeLogical a physical orientation
G4LatticePhysical* GePhysical = new G4LatticePhysical(GeLogical);
GePhysical->SetMillerOrientation(1,0,0);
LM->RegisterLattice(GePhys, GePhysical);

// NOTE:  Above registration can also be done in single step:
// G4LatticlePhysical* GePhysical = LM->LoadLattice(GePhys, "Ge");

//
// Aluminum - crystal end caps. This is where phonon hits are registered
//
G4VSolid* fAluminumSolid = new G4Tubs("aluminiumSolid",0.*cm,3.81*cm,0.01*cm,
                                      0.*deg, 360.*deg);

G4LogicalVolume* fAluminumLogical =
  new G4LogicalVolume(fAluminumSolid,fAluminum,"fAluminumLogical");
G4VPhysicalVolume* aluminumTopPhysical = new G4PVPlacement(0,
  G4ThreeVector(0.,0.,1.28*cm), fAluminumLogical, "fAluminumPhysical",
  worldLogical,false,0);
G4VPhysicalVolume* aluminumBotPhysical = new G4PVPlacement(0,
  G4ThreeVector(0.,0.,-1.28*cm), fAluminumLogical, "fAluminumPhysical",
  worldLogical,false,1);
```

Non-Ideal Phonon Losses in Films

- G4CMP has never explicitly dealt with sub-gap phonon losses in superconducting films, because it was largely irrelevant to our single-film implementation

- There are a couple of mechanisms we need to account for
    - Interface-scattering losses - can be implemented with a macro by changing loss at boundaries
    - Ultrasonic attenuation - this will correlate with reduced qp density but has temperature dependence as well. It could be easy to implement
    - Grain-boundary scattering within films - we can base these models on those constructed for thermal conductance, but it's unclear how to treat final states. Work is needed.

$$\tau_{phs}^{-1} \approx \frac{\tau_0^{-1}}{\pi^{3/2}} \sqrt{\frac{2k_bT}{\Delta(0)}} x_{qp} \left(1 - e^{-\omega/k_bT}\right)$$



$$\lambda_{gb} = \lambda_{gb,0} \frac{\omega_D}{\omega}$$

Phonon Transport Planned Upgrades

- Iteratively work towards more complete reflection model
  - Incorporate angle and medium dependence
  - Incorporate polarization dependence
  - Properly deal with reflection back into the substrate
  - Verify that these changes match existing validation data from the Si/Ge detectors we use to benchmark simulations

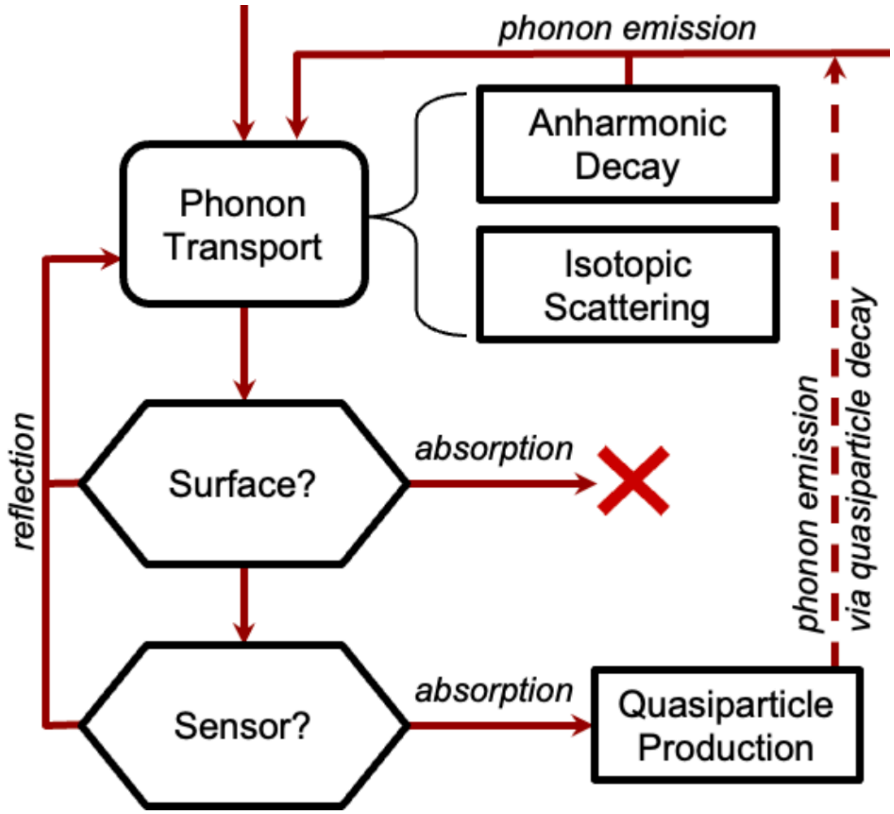
- Improve demos for different types of phonon modeling applications - this may need to largely be a community driven process
  - Single crystal with multiple types of surface films
  - Demonstrate changing thickness and reflection probabilities in macros for automated parameter tuning
  - Other suggestions?

- Aside from reflection, the physics processes are mature, we just need a larger code-based to draw on
  - As people add substrates, some detail of how that was done should be included in G4CMP

Quasiparticles Don't Exist in G4CMP

- When a phonon hits a film and is absorbed, the following occurs:
  - Absorption probability calculated based on phonon lifetime in the film and film thickness
  - If absorbed, KaplanQP is called. This can emit phonons (sub-gap) back into the substrate, and returns 'total energy deposited'
  - Occasionally some above-gap phonon emission can occur based on random angle - unclear how robust this is

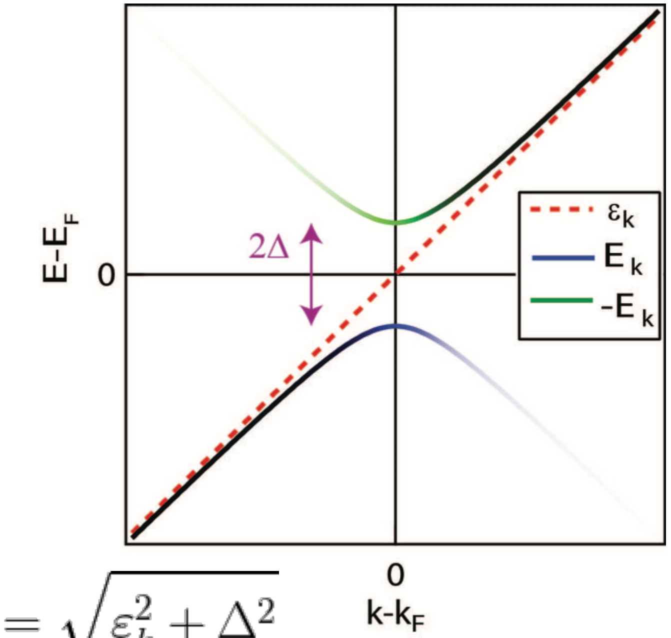
- This requires the user to convert back into quasiparticle number and model diffusion separately, despite the fact that all of the physics is implement in KaplanQP



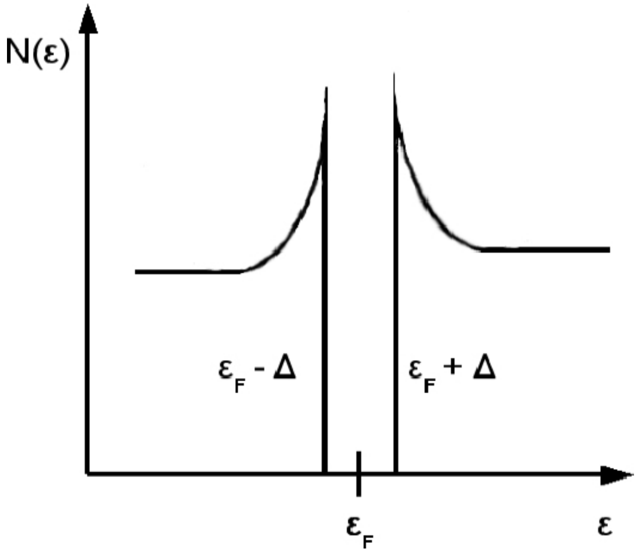
How Can We Model Quasiparticles?

- Our model of hole diffusion in semiconductors is almost what would be needed to implement quasiparticle diffusion, except that
  - The non-linear dispersion relation can’t be naturally implemented outside of KaplanQP
  - Coherence and DOS effects can’t be naturally included
  - The momentum conservation equations will look different (electrons all have large finite k-vector)

- If we were to port the rate equations from KaplanQP into phonon emission equations, like we do in the substrate, the rest of the simulation would look fairly similar up to the conditions enforcing momentum and energy conservation

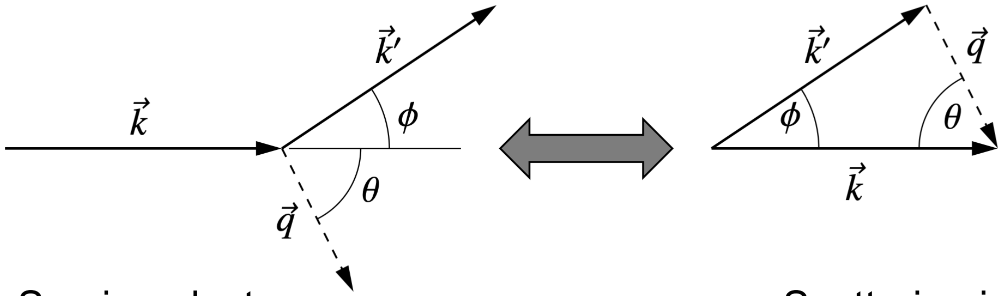


$$E_k = \sqrt{\varepsilon_k^2 + \Delta^2}$$



Phys Rev D 107, 076015 (2023)
https://github.com/benvlehmann/scdc

Implementing Scattering in Metals



$$\gamma \equiv \sqrt{\frac{\frac{1}{2} m_* c_s^2}{\Delta}}$$

Scattering in Semiconductors

$$\cos\phi = \frac{k^2 - 2k_L(k\cos\theta - k_L) - 2(k\cos\theta - k_L)^2}{k\sqrt{k^2 - 4k_L(k\cos\theta - k_L)}}$$

Scattering in Superconductors

$$\cos\theta_q = \frac{\omega_q^2 + 4\gamma^2\Delta\left[s\sqrt{(E_{\mathrm{QP}}^2 - \Delta^2)} - s'\sqrt{(E_{\mathrm{QP}} - \omega_q)^2 - \Delta^2}\right]}{4\gamma\omega_q\left[E_{\mathrm{F}}\Delta + s\Delta\sqrt{(E_{\mathrm{QP}}^2 - \Delta^2)}\right]^{1/2}}$$

- The differential scattering rate in k is very similar to that used already in G4CMP - the main difference is the directionality of the emission
- The scattering rate is the same already implemented in KaplanQP, differing just by increase in DOS and coherence factors
- Changes needed to add ‘metal’ and ‘superconductor’ classes can be simplified to the general superconductor case, and just involve changing k-vector selection rules relative to semiconductor assumptions

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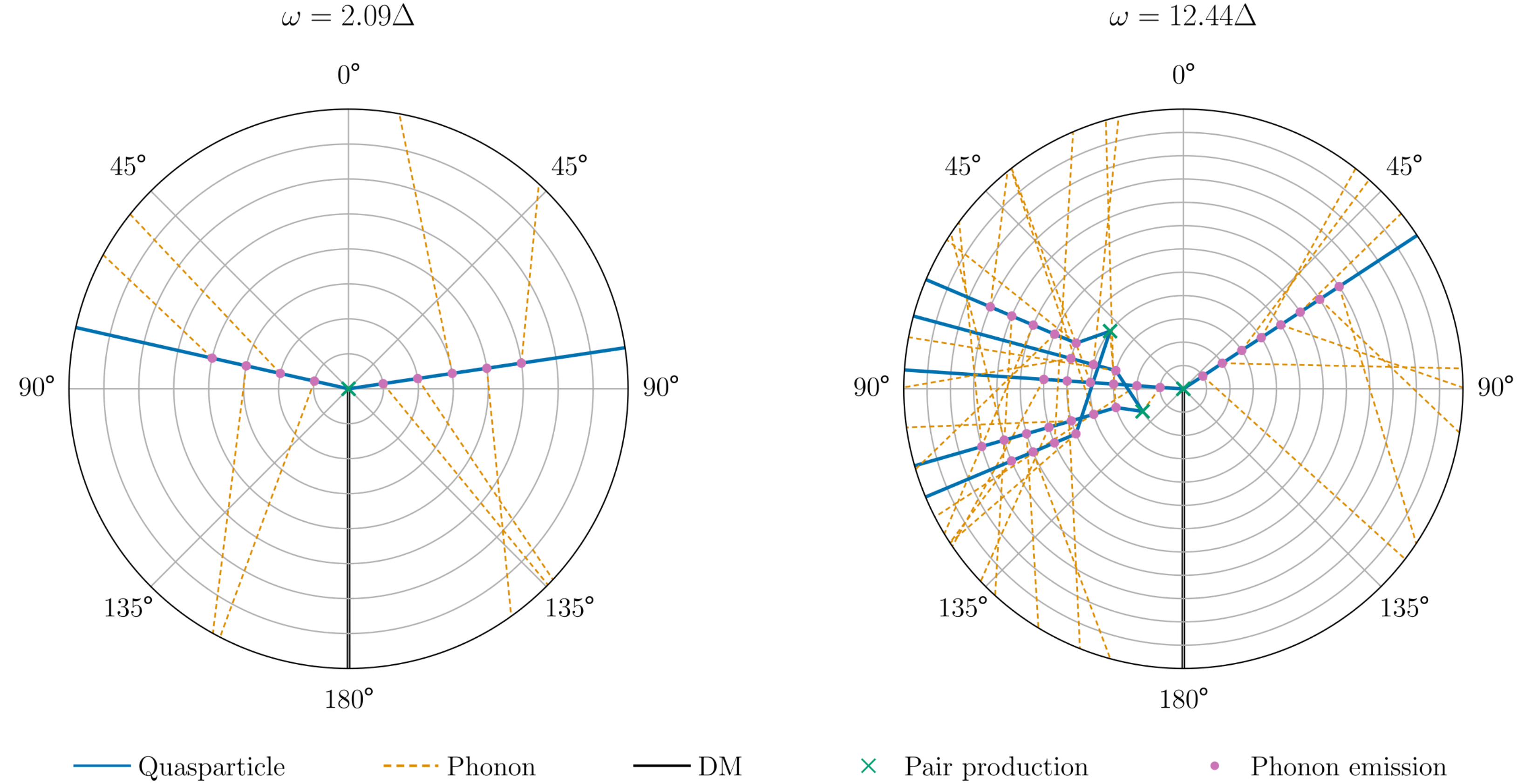
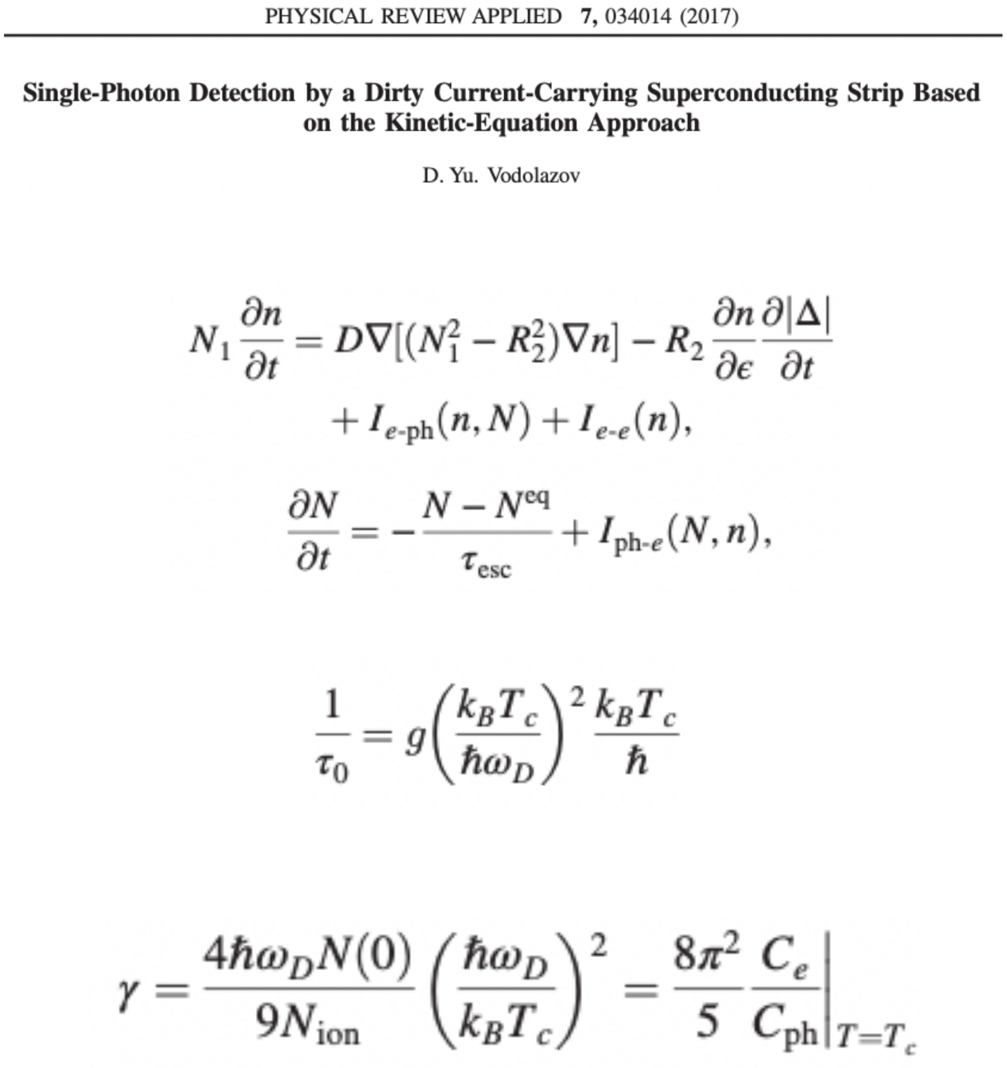
How Do We Extend KaplanQP?



- We’ve implemented this in the SCDC package on github as part of modeling anisotropic quasiparticle dynamics in a dark matter context, but similar hit diagrams can be drawn as we do for phonon down-conversion in crystals.

Nanowire Hotspot Model - Possible Diffusion Model?

- The microphysical model for the hotspot generation and decay has gotten more quantitative recently - until the mid 2010s, there was not a self-consistent model for the factors driving the bubble dynamics
- Luckily for us, these are the same dynamics as earlier in the lecture with some time and spatial dependence added to create a set of coupled kinetic equations
    - D, the diffusivity of the electrons, figures prominently in the source term - too large and they will quickly diffusion before creating a localized spot
- The characteristic timescale is again defined by g (electron-phonon coupling constant) and Tc cubed
- An additional parameter is important to understanding how quickly the phonons cool the electron bubble, which determines the efficiency with which the nanowire can be driven normal



PHYSICAL REVIEW APPLIED **7,** 034014 (2017)

Single-Photon Detection by a Dirty Current-Carrying Superconducting Strip Based on the Kinetic-Equation Approach

D. Yu. Vodolazov

$$N_1 \frac{\partial n}{\partial t} = D\nabla[(N_1^2 - R_2^2)\nabla n] - R_2 \frac{\partial n}{\partial \epsilon}\frac{\partial|\Delta|}{\partial t} + I_{e\text{-ph}}(n, N) + I_{e\text{-}e}(n),$$

$$\frac{\partial N}{\partial t} = -\frac{N - N^{\mathrm{eq}}}{\tau_{\mathrm{esc}}} + I_{\mathrm{ph}\text{-}e}(N, n),$$

$$\frac{1}{\tau_0} = g\left(\frac{k_B T_c}{\hbar\omega_D}\right)^2 \frac{k_B T_c}{\hbar}$$

$$\gamma = \frac{4\hbar\omega_D N(0)}{9N_{\mathrm{ion}}}\left(\frac{\hbar\omega_D}{k_B T_c}\right)^2 = \frac{8\pi^2}{5}\frac{C_e}{C_{\mathrm{ph}}}\bigg|_{T=T_c}$$

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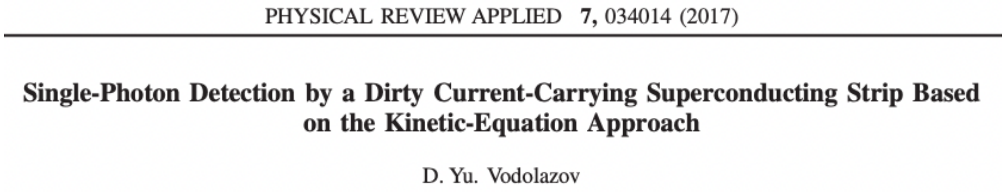

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$$\frac{\partial N}{\partial t} = -\frac{N - N^{\mathrm{eq}}}{\tau_{\mathrm{esc}}} + I_{\mathrm{ph}\text{-}e}(N,n),$$

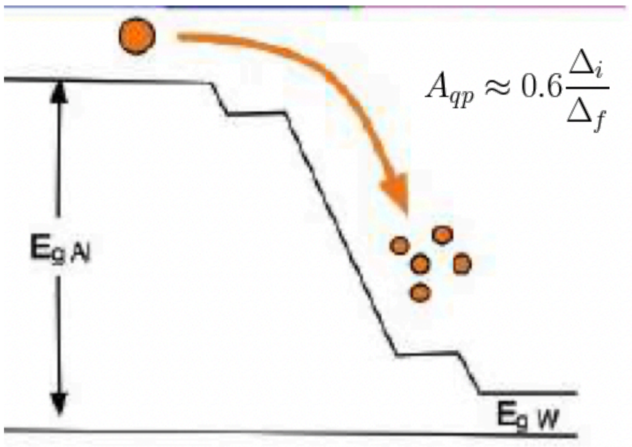
$$\tau_0 = Z_1(0)\hbar/2\pi b(kT_c)^3$$

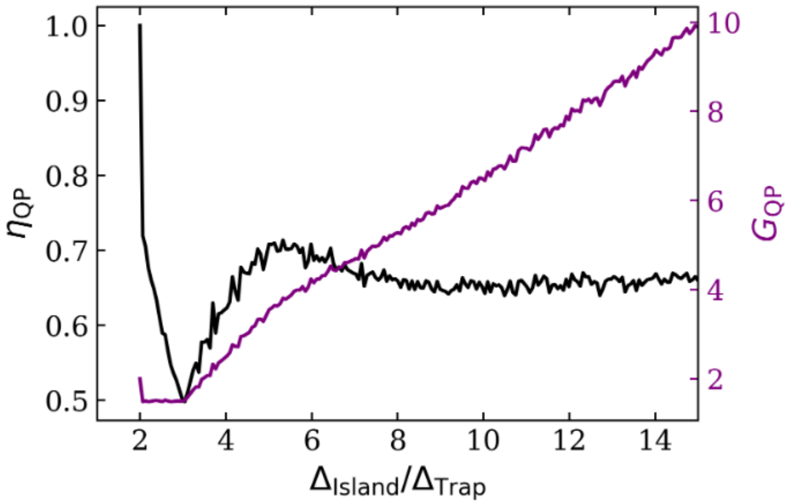
$$\gamma = \frac{4\hbar\omega_D N(0)}{9N_{\mathrm{ion}}}\left(\frac{\hbar\omega_D}{k_B T_c}\right)^2 = \frac{8\pi^2}{5}\frac{C_e}{C_{\mathrm{ph}}}\bigg|_{T=T_c}$$

https://arxiv.org/abs/2310.01345

Modeling QP Trapping and Amplification

- If we can implement quasiparticles and phonons in G4CMP, we can add diffusion - this means modeling trapping and QP amplification
- Whether this should be done in G4CMP or in a post-processing script is another question, but traps and spatial variations in gap seem to be common features we would all like to simulate
- Modeling trapping probability is an open problem - we have limited data to benchmark the trapping probability - so it's likely G4CMP can help us learn more about how to optimize QP traps
    - We could include flux traps and normal metal/low-gap traps to separate the QP lifetime and effective trapping length into distinct parts of the simulation





G4CMP Adjacent Tools

- There are a number of common modeling steps that are likely beyond the scope of G4CMP but could be worked on collaboratively by the G4CMP community
  - As an example, we have TES and charge readout response tools that use G4CMP outputs for detector response modeling in SuperCDMS, but they are not part of G4CMP

- We don’t have specific plans, but our hope is this community will find ways to develop post-processing layers for G4CMP alongside G4CMP development
  - Workflow for implementing new materials in G4CMP, both crystals and metal films
  - Workflow for implementing complex film geometry from GDS file
  - Response modeling for simple resonators/qubit geometries
  - Other needs identified by G4CMP community

Topics for Discussion

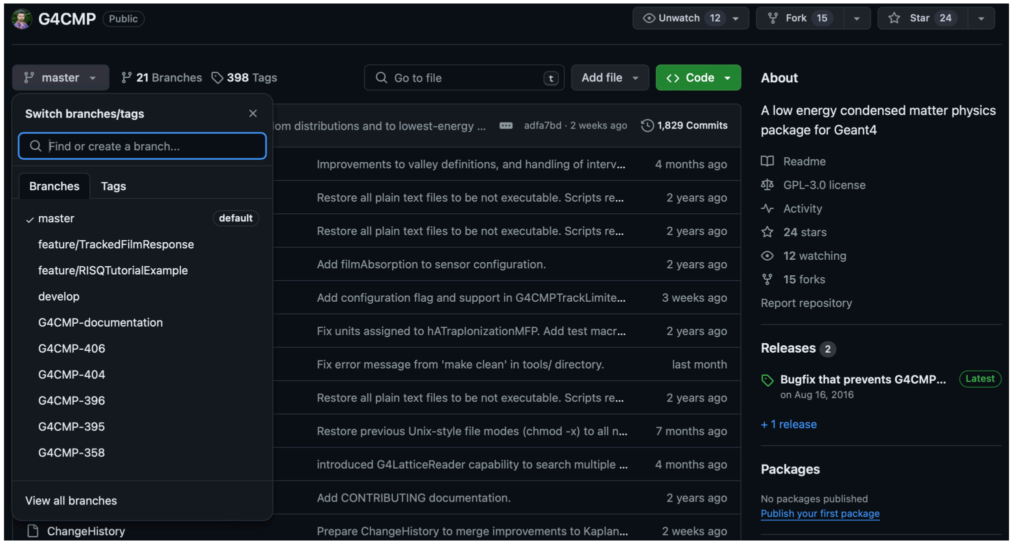
- Not a complete list, but some common themes that seem to come up frequently:
  - What demos are useful to show how to properly implement models in G4CMP (can also be vanilla GEANT demos that integrate G4CMP functionality)?
  - What other materials might we want? Do we also want a standard set of superconducting and normal films?
  - Do we care about optical phonons?
  - How realistic do we need phonon dynamics to be?
  - What aspects of QP diffusion do we want to include in G4CMP? How far into our detector response can this realistically extend?

- How do we organize G4CMP development going forward - how can we incentivize people to help implement new features that benefit the rest of the community?

G4CMP Development: How and Where

- Most of you will have found G4CMP via GitHub, but is has a weird hybrid existence between CDMS and public code
    - Issue tracking is managed within SLAC Jira, active developers are associated with CDMS
    - Going forward, we need to migrate these issues to Github and institute some limited issue tracking (we don't have the level of support to respond to all issues submitted by the community, but it's good to show what has been identified and what we're working on)

- One outcome from this workshop is to try to establish a set of people interested in helping with ongoing G4CMP development that can help setup this infrastructure


G4CMP Public

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master · 21 Branches · 398 Tags · Go to file · t · Add file · Code

Switch branches/tags

Find or create a branch...

Branches · Tags

- ✓ master (default)
- feature/TrackedFilmResponse
- feature/RISQTutorialExample
- develop
- G4CMP-documentation
- G4CMP-406
- G4CMP-404
- G4CMP-396
- G4CMP-395
- G4CMP-358

View all branches

om distributions and to lowest-energy ... · adfa7bd · 2 weeks ago · 1,829 Commits

Improvements to valley definitions, and handling of interv...	4 months ago
Restore all plain text files to be not executable. Scripts re...	2 years ago
Restore all plain text files to be not executable. Scripts re...	2 years ago
Add filmAbsorption to sensor configuration.	2 years ago
Add configuration flag and support in G4CMPTrackLimite...	3 weeks ago
Fix units assigned to hATraplonizationMFP. Add test macr...	2 years ago
Fix error message from 'make clean' in tools/ directory.	last month
Restore all plain text files to be not executable. Scripts re...	2 years ago
Restore previous Unix-style file modes (chmod -x) to all n...	7 months ago
introduced G4LatticeReader capability to search multiple ...	4 months ago
Add CONTRIBUTING documentation.	2 years ago
ChangeHistory · Prepare ChangeHistory to merge improvements to Kaplan...	2 weeks ago

About

A low energy condensed matter physics package for Geant4

- Readme
- GPL-3.0 license
- Activity
- 24 stars
- 12 watching
- 15 forks

Report repository

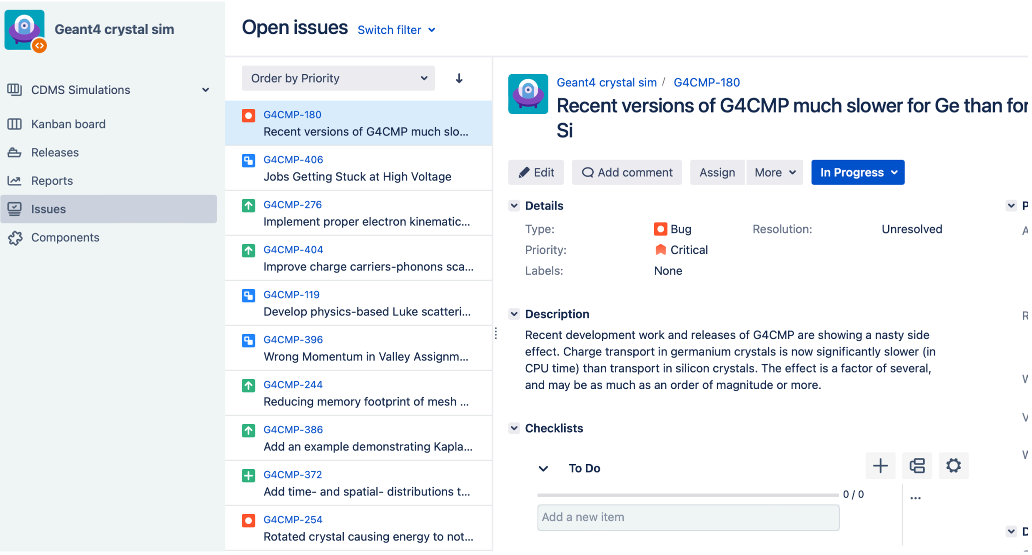
Releases 2

Bugfix that prevents G4CMP... Latest
on Aug 16, 2016

+ 1 release

Packages

No packages published
Publish your first package


Geant4 crystal sim

- CDMS Simulations
- Kanban board
- Releases
- Reports
- Issues
- Components

Open issues · Switch filter

Order by Priority

- G4CMP-180 Recent versions of G4CMP much slo...
- G4CMP-406 Jobs Getting Stuck at High Voltage
- G4CMP-276 Implement proper electron kinematic...
- G4CMP-404 Improve charge carriers-phonons sca...
- G4CMP-119 Develop physics-based Luke scatteri...
- G4CMP-396 Wrong Momentum in Valley Assignm...
- G4CMP-244 Reducing memory footprint of mesh ...
- G4CMP-386 Add an example demonstrating Kapla...
- G4CMP-372 Add time- and spatial- distributions t...
- G4CMP-254 Rotated crystal causing energy to not...

Geant4 crystal sim / G4CMP-180

Recent versions of G4CMP much slower for Ge than for Si

Edit · Add comment · Assign · More · In Progress

Details

Type: Bug
Priority: Critical
Labels: None
Resolution: Unresolved

Description

Recent development work and releases of G4CMP are showing a nasty side effect. Charge transport in germanium crystals is now significantly slower (in CPU time) than transport in silicon crystals. The effect is a factor of several, and may be as much as an order of magnitude or more.

Checklists

To Do · 0 / 0

Add a new item

Summary

- G4CMP functionality is beginning to expand, and the increased (diversified) user base is part of the reason
- We can now simulate non-ideal effects we couldn't a few years ago - charge trapping, sub-gap phonon emission, new materials - but we can keep pushing to improve implemented physics
- With a broader range of devices, and more complementary validation data, it's likely we can more robustly constrain new processes implement in G4CMP