Electron Transportation in Geant4 Condensed Matter Physics Simulation for Use in Searches for Dark Matter

Texas A&M University

Iman Ataee Langroudy
Thesis Defense

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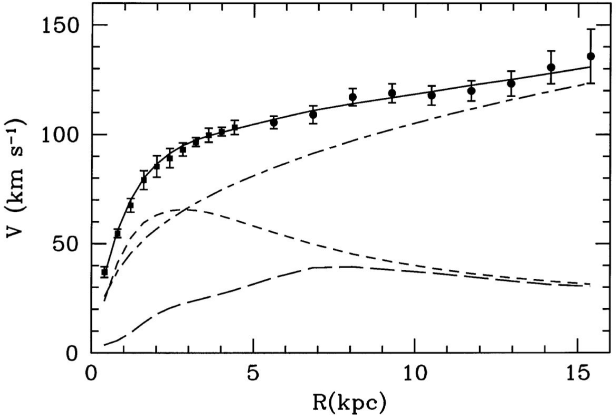
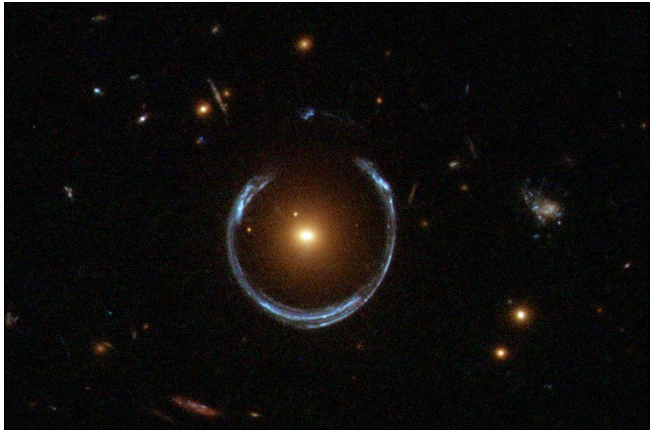
Outline

- Introduction and Motivation
    - Dark Matter and Super Cryogenic Dark Matter Search Experiment (SuperCDMS)
    - Charge Arrival Distributions on the Detector Surfaces
    - Thesis Goals
    - SuperCDMS Detector Simulations
- Dominant Effects in the Electron Transportation in a Semiconductor Crystal
    - Energy-Momentum Relationship
    - Electric Field
    - Scattering Effects
- Simulating the Dominant Effects with a Toy Simulation
    - Trajectories
    - Arrival Positions at the Top Surface
- Geant4 Condensed Matter Physics (G4CMP) Addon
    - Overview
    - Results and Comparison with Experiment
- Future Works and Conclusion

The Mystery of Dark Matter

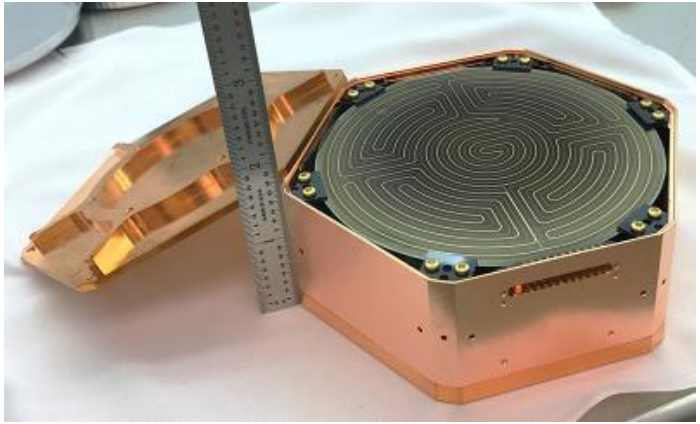
- Observed gravitational effects in the universe cannot be fully explained by visible matter alone
- Dark matter is proposed to account for this "missing" mass, influencing galaxy formation and cosmic structure
  - Stars at galaxy edges move faster than predicted if only visible matter is considered (top figure)
  - Observed gravitational lensing patterns (Einstein rings) around distant galaxies are different than calculated from the visible matter
- Simplest solutions: Weakly Interacting Massive Particles (WIMPS) are hypothetical particles that barely interact with normal matter, making them nearly invisible

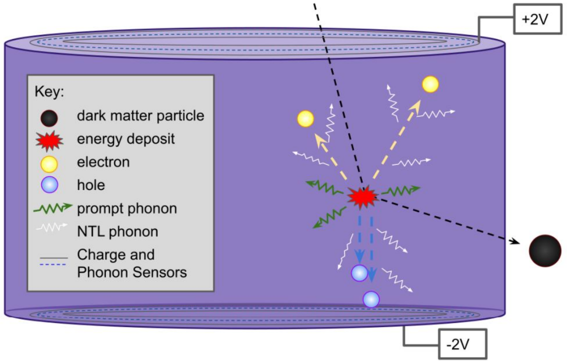




Super Cryogenic Dark Matter Search Experiment (SuperCDMS)

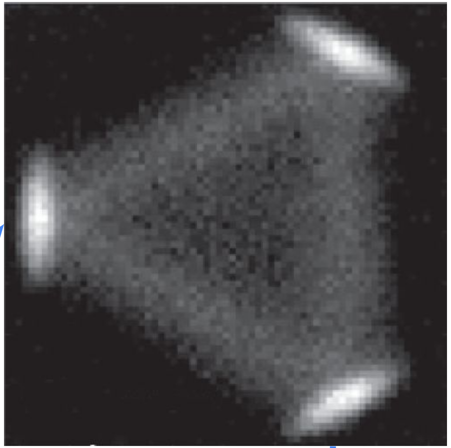
- The Super Cryogenic Dark Matter Search Experiment (SuperCDMS) is designed to directly detect particle dark matter using silicon or germanium detectors at millikelvin temperatures to measure small energy particle interactions
- When either standard model particle or dark matter particles hit a detector, they deposit energy and excite electrons to form an electron-hole pair and emit phonons
- Electrons get accelerated and travel through the detector, scatter, and emit phonons, until they hit the sensors
- We can calculate the energy of the incident particle using the energy that the phonons and charges deposit on sensors



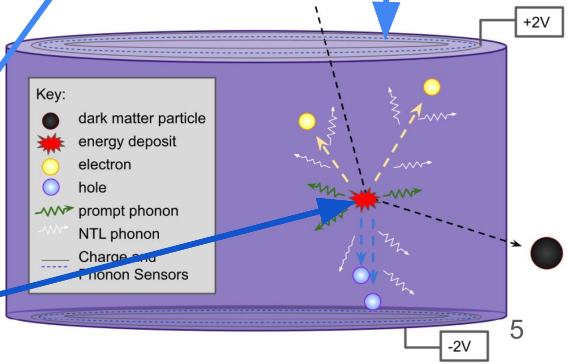


Physics Goal: Understanding of Charge Arrival Distributions on the Detector Surfaces

- In a detector, what we see are the patterns that electrons, holes, and phonons form on the sensors, at the top surface, which we call "data"
- We need to have a fidelity set of expectations of how the detector responds to a complex interaction from a dark matter particle if we want to be able to separate from noise or mismeasured background events
- Simple controlled case: observed electron arrival positions on the top surface for a set of electrons starting inside the detector with exactly the same position and energy, and moving under a uniform Z electric field
- The patterns in single-crystal semiconductors are completely different from what we'd expect for an electron in a vacuum, or from typical scattering in a material



Si (111)



We need to interpret these patterns

If we want to understand what happened here

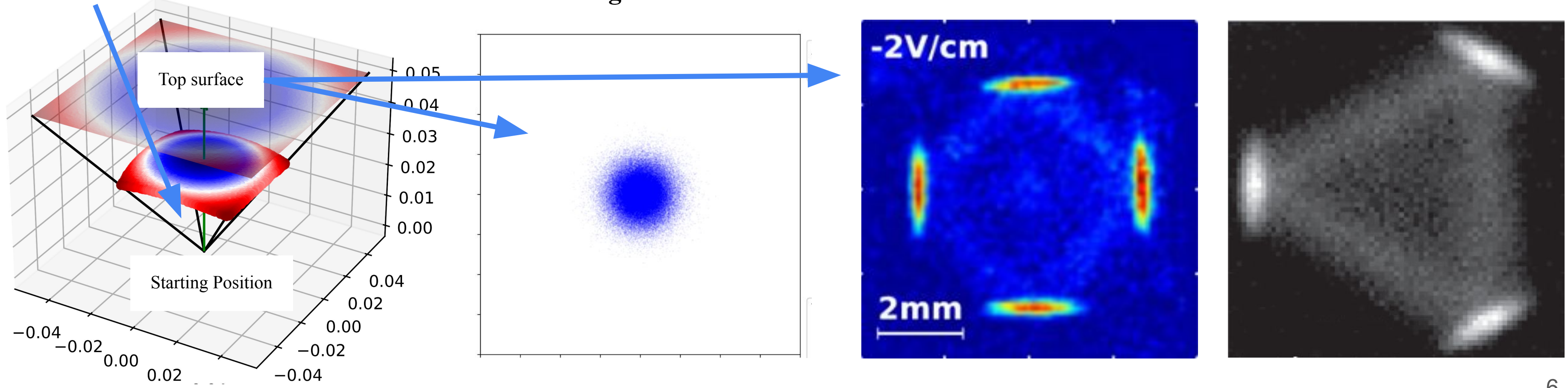
Understanding of Charge Arrival Distributions on the Detector Surfaces

- The patterns that we see are VERY different between vacuum, silicon, and germanium for reasons that are highly non-intuitive even for the simplest cases

Set of electrons from a single point, all with the same energy but starting in random directions.

What we expect to observe if the set of electrons were moving under a voltage in vacuum

What we observe when the set of electrons moved under a voltage in germanium (left) and silicon (right)



Thesis Goals

- Our goal is to have high-fidelity simulations of electron transport[1] that provide accurate predictions of the charge and phonon arrival distributions at the sensors of semiconductor detectors
- Since doing so will be non-trivial as many of the effects are non-intuitive, we will do this in a number of steps:
  a. Describe the dominant effects (mostly due to the wave-like nature of electrons)
  b. Develop methods for particle-like modeling to be incorporated into powerful standard simulation frames such as Geant4
  c. Implement a standalone simulation (toy model) to provide intuition and expectations for what the main simulation results should look like
  d. Implement all the effects in the full simulation framework and compare the results to both our expectations and the experimental data

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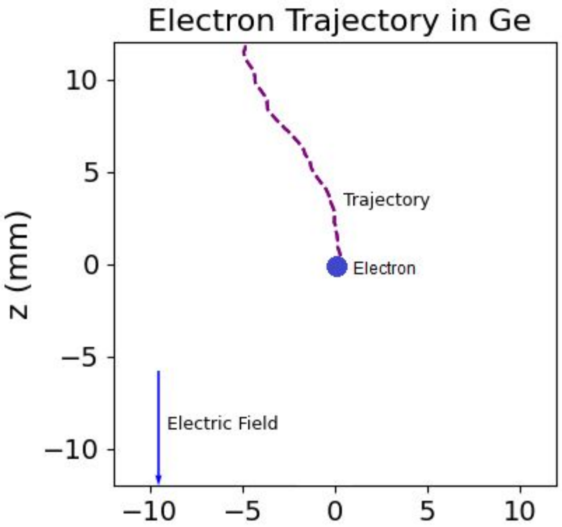
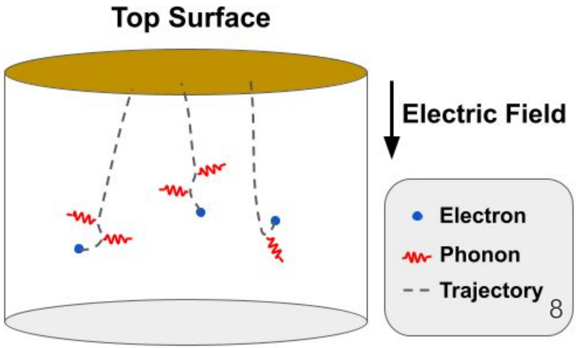
[1] improve the previous simulation framework that was not matching our expectations and understanding

Dominant Effects on Electron Transport in a Semiconductor Crystal

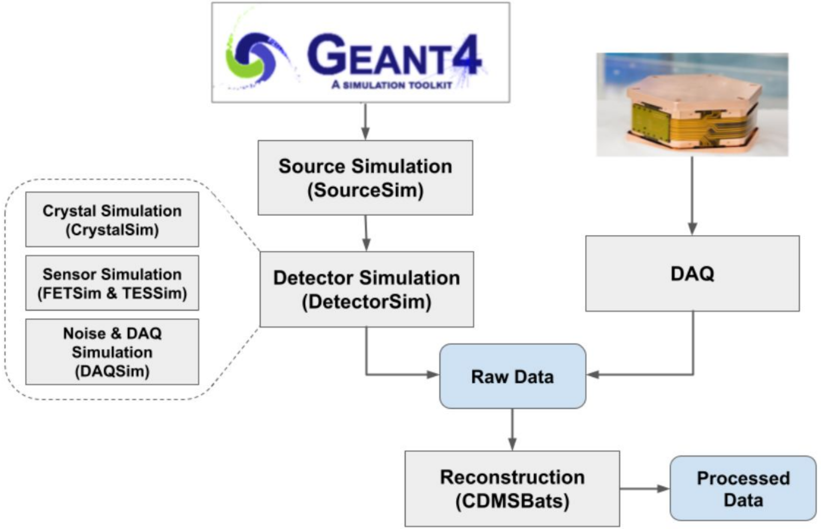
- There are multiple competing dominant effects, most of which are due to the wave-like, quantum-mechanical nature of electrons in a crystal lattice:
  - **Effect 1:** There are certain directions in which same-energy electrons move more slowly; these are referred to as "valleys"
  - **Effect 2:** Charges behave “oddly” in an electric field in semiconductor crystals: The direction and magnitude of any acceleration is not only a function of an external force, but is also a function of the crystal orientation
  - **Effect 3:** Charges can scatter within the crystal either from the lattice or other particles and produce phonons
- Using our understanding and our modeling, we can build a high quality simulation for use in the search for dark matter (and other areas)





SuperCDMS Detector Simulations

- Geant4 serves as the foundation of the SuperCDMS detector simulation as it provides a widely validated toolkit for modeling particle propagation and interactions, in custom detector geometries
- Since it represents charged particles using a classical, point-like description and does not natively support the quantum-mechanical behavior of charges in a semiconductor crystal, we will need a semi-classical approximation to model these effects within the Geant4 infrastructure



GEANT4
A SIMULATION TOOLKIT

Source Simulation (SourceSim)

Detector Simulation (DetectorSim)

Crystal Simulation (CrystalSim)

Sensor Simulation (FETSim & TESSim)

Noise & DAQ Simulation (DAQSim)

DAQ

Raw Data

Reconstruction (CDMSBats)

Processed Data

- This additional modeling is included in the Geant4 Condensed Matter Physics (G4CMP) add on package

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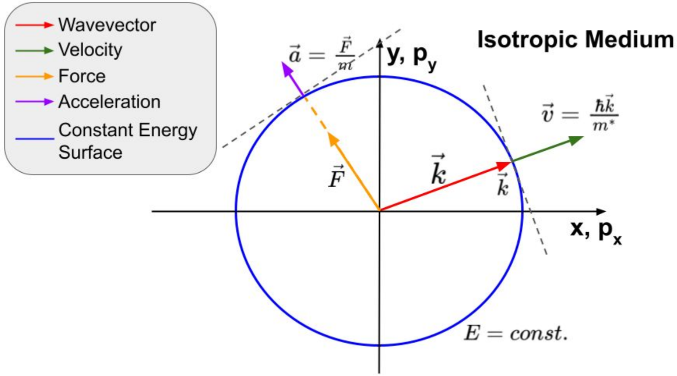
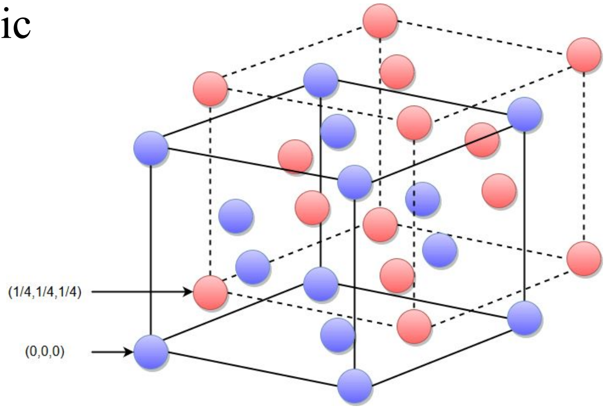
Charge Propagation in an Isotropic Medium (Simplest Case)

- Since the dominant effects are non-intuitive for the wave-like motion of electrons, we start with the simple case of particle motion in a vacuum where we have good intuition and build up from there
- The figure shows a two-dimensional image of the relationship between the kinetic energy of a particle in an isotropic medium and its wavevector
  - Same energy electrons have same wavevector and velocity magnitude
  - The velocity and acceleration are in the same direction as the wavevector and force respectively



The Crystal Lattice Affects the Allowed Energy in Different Directions

- Semiconductor crystals have an anisotropic lattice structure which gives different directions in space different properties
- Both silicon and germanium are special because they are periodic in physical space which leads to a periodic potential in the Schrödinger equation
- We can use Bloch's theorem which takes advantage of the periodicity of the potential in physical space to determine the electron's energy periodicity in wavevector[1] space
  - The allowed energies are continuous, but are only periodic energy bands with extrema in wavevector space



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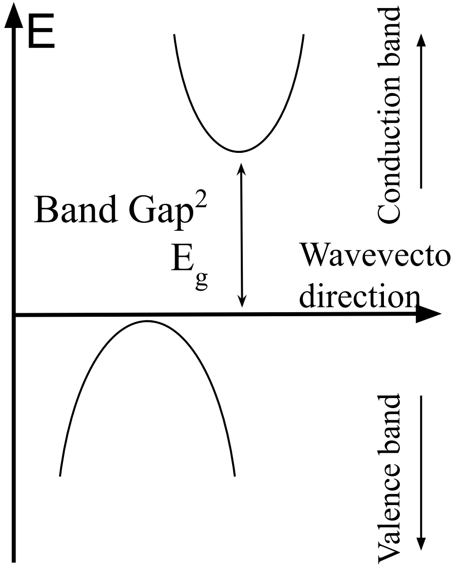
1. Wavevector Definition

Energy is Different in Different Directions

- Extrema in the energy bands means minimums in the conduction bands (free electrons) and maximums in the valence bands (free holes) in phase space
- Both are direction dependent, so we refer to the directions of the lowest energy levels in the conduction bands as **Valleys**[1]
  - Six valleys in Silicon
  - Eight valleys in Germanium
- Note that the figure here is just a simplified version to help with our intuition



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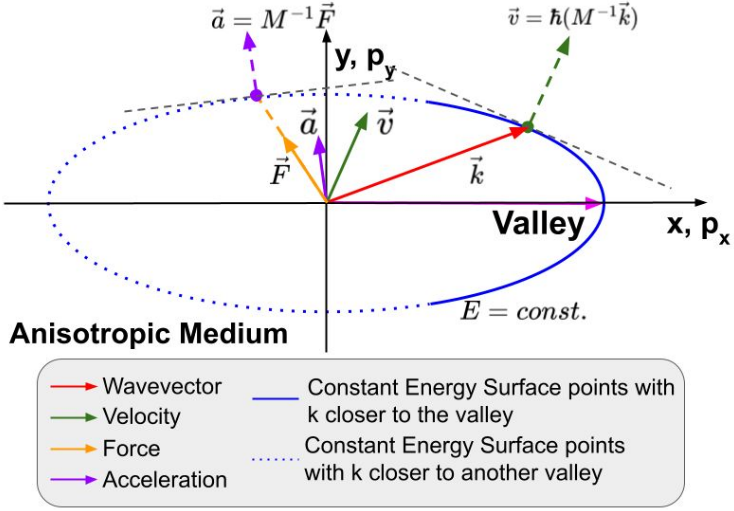
1. Notable Directions in the Conduction Band
2. Low Temperature Band Gaps

Modeling the Motion of Charges in the Crystal Without Derivation

- It turns out[1] we can build a particle-like modeling and describe the trajectories as particle-like motion in a vacuum but where different directions have different "mass"

Free Electron	$E_{kin} = \frac{1}{2}\frac{p^2}{m_0} = \frac{1}{2}m_0 v^2$	$v = \frac{p}{m_0} = \frac{\hbar k}{m_0}$	$a = \frac{F}{m_0}$
Electron in Crystal	$E_{kin} = \frac{1}{2} < p\|M^{-1}\|p >= \frac{1}{2} < v\|M\|v >$	$v = M^{-1}p = M^{-1}\hbar k$	$a = M^{-1}F$

- The mass term in the equations becomes a 3x3 matrix which essentially includes the information about the crystal: Refer to this as **Mass Tensor**, ***M***
- In an anisotropic medium, the velocity and acceleration directions are governed by the mass tensor and are not necessarily in the same direction as the wavevector and force



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1. All the math and modeling is done in chapters 2 and 3, and the results are summarized here

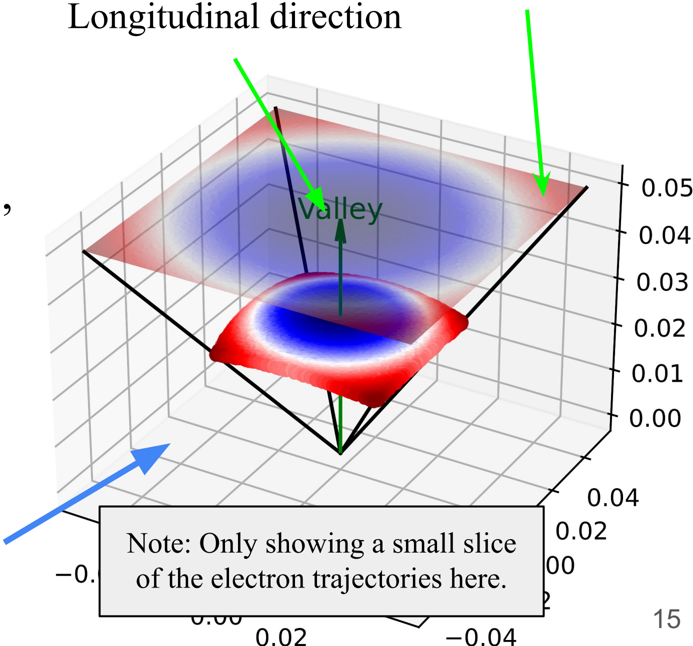
Mass Tensor and Momentum Magnitude for a Single Valley

$$M = \begin{bmatrix} m_l & 0 & 0 \\ 0 & m_t & 0 \\ 0 & 0 & m_t \end{bmatrix}$$

- We can consider all motion local, and move to a frame where the x-axis is along the valley direction
  - We refer to the valley direction as longitudinal, and the other two as being transverse
  - In this frame the mass tensor becomes diagonalized and well described by two different masses. Previous experiments have measured these effective masses
- As the longitudinal mass is bigger than the transverse mass, same energy electrons with a speed (or momentum) direction closer to the valley have a smaller speed (momentum) magnitude

Bigger Speed
Transverse direction

Smaller Speed
Longitudinal direction

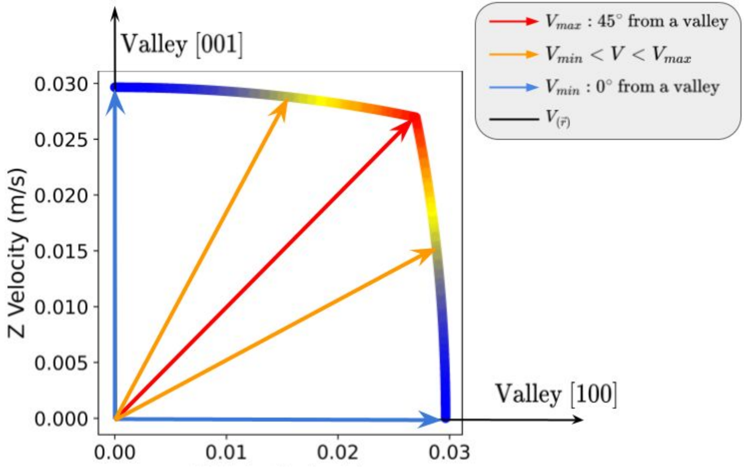


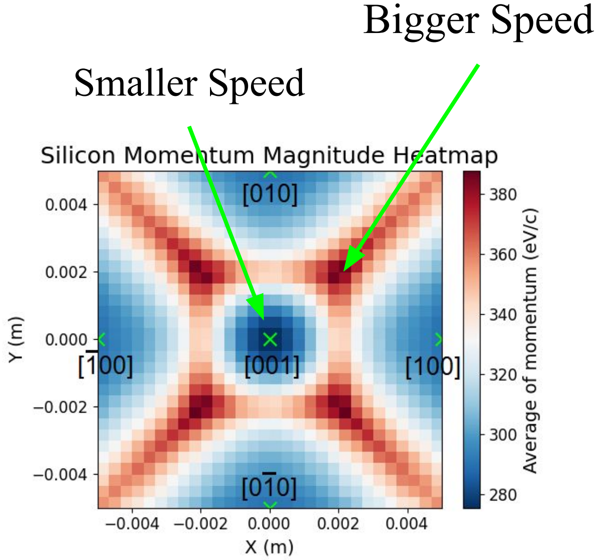
Note: Only showing a small slice of the electron trajectories here.

For the rest of the the talk, we will show many plots with similar setup: A set of monoenergetic elections all emanating from a single point in random directions and we study what we see on the surface

Moving to More Than One Valley

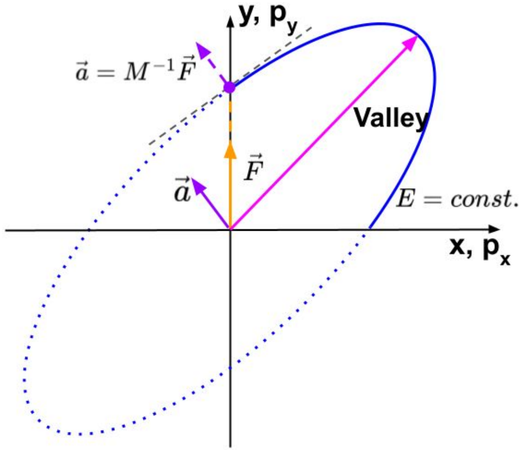
- The top figure shows the electron speed within the crystal as a function of it's direction between two valleys
  - Note the maximum and minimum as a function of direction relative to the valley
- The bottom figure again shows the momentum distribution at the top surface when we include all Silicon valleys

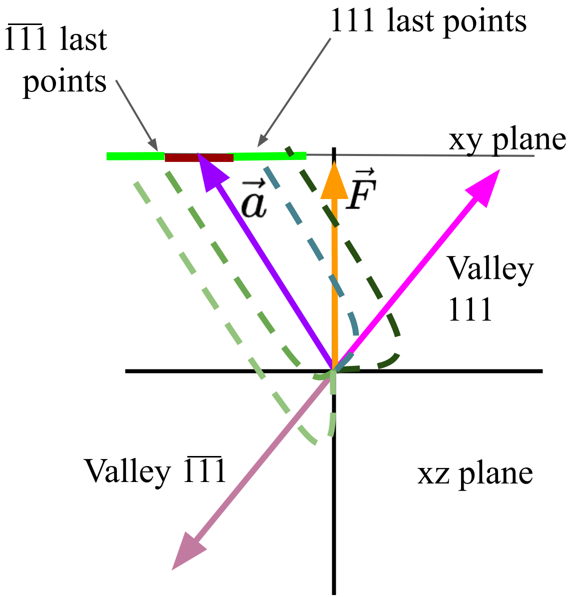




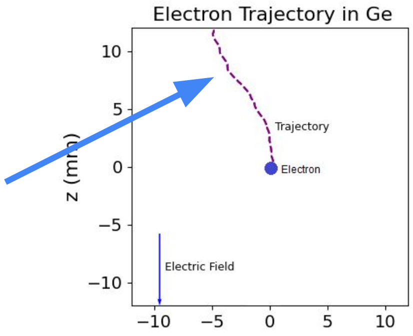
Charge Transport Under an Electric Field

- When there is a force in the semiconductor crystal the acceleration and force are not necessarily in the same direction
- The bottom plot shows the simple case of a germanium crystal where the force is in a direction different than a valley (like in the CDMS experiment) => the acceleration and trajectories from the origin are shown as solid and dashed lines
- For valleys on the same axis but in opposite directions, the electrons in both valleys will have the same acceleration and will end up in a similar location on the top surface



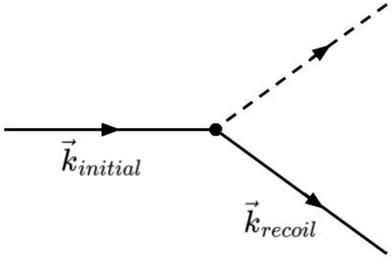


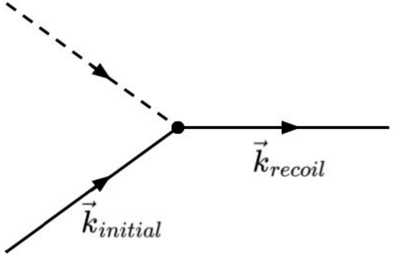
- Getting accelerated in a different direction
- Has scattering, which we talk about next

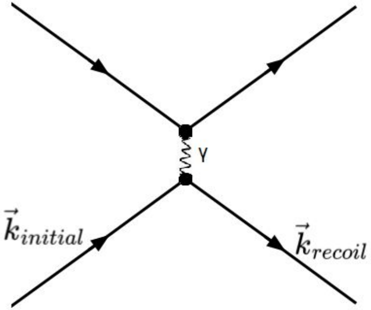


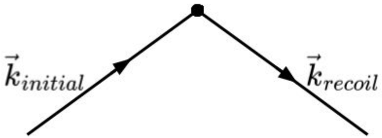
Scattering in a Semiconductor Crystal

- In addition to transport in the electric field, scatterings in the crystal can have a large impact on the full path
- While there are many types of scattering, we start by listing the primary first-order effects and then focus on the dominant ones:
  1. Charges scatter off of an atom and emit a phonon
     - **Acoustic phonon scatterings** that emit low energy phonons
     - **Optical phonon scattering** that emit high energy phonons
  2. Charges encounter a phonon in the lattice and absorb it, changing directions
  3. Charges scatter off of another charge and trade some energy in the process
  4. Charges encounter an impurity in the crystal structure which causes an elastic scattering
- Depending on if the electron’s valley changes or not, we call it an **intervalley** or **intravalley** scattering respectively

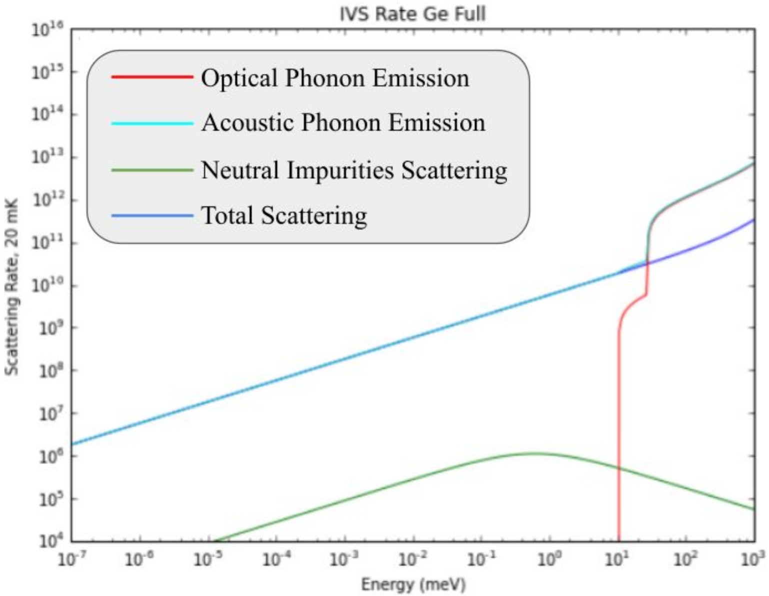








Scattering in a Semiconductor Crystal



At low energies/temperatures the complexity is significantly reduced:

- The phonon absorption and charge-charge scatterings are rare due to low population of phonons and free charges
- Optical phonon emissions can still happen, but only at higher energies (often intervalley)[1]

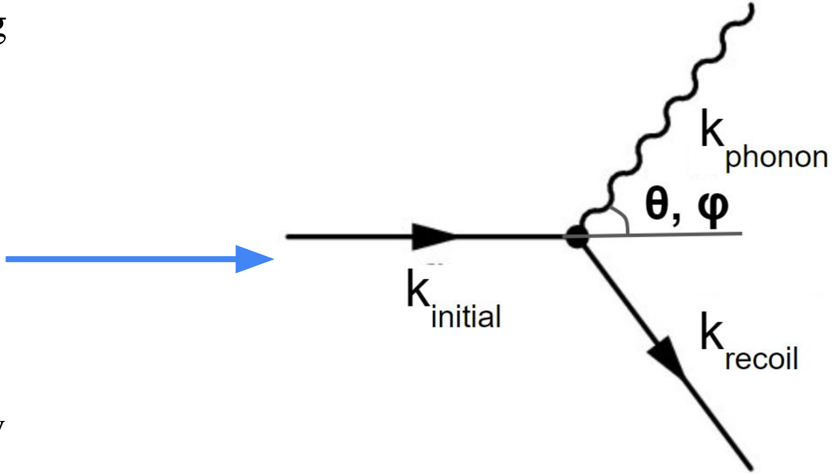
To a good degree of approximation, the intravalley acoustic phonon emission scatterings dominates all scatterings while impurity scattering dominates the intervalley scatterings

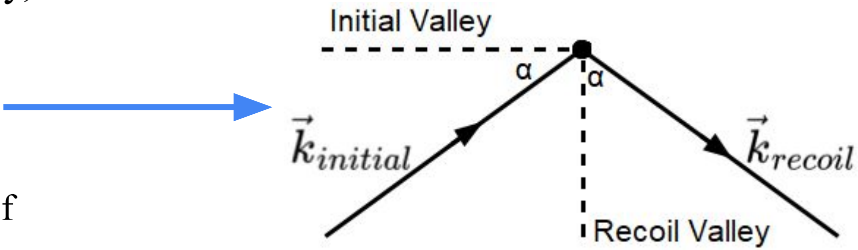
1. More details in the backup

Effective Scattering Model

For our work we will approximate all scatterings as being one of the two types shown on the right:

- **Intravalley Scattering:** Electron stays in the same valley and a phonon is emitted
  - Rates and kinematics are calculated microscopically using first principles as a function of charge's energy
- **Intervalley scatterings:** Electron scatters elastically, changing the valley while preserving its angle with the valley
  - Rates are calculated probabilistically as a function of voltage (macroscopically)[1]





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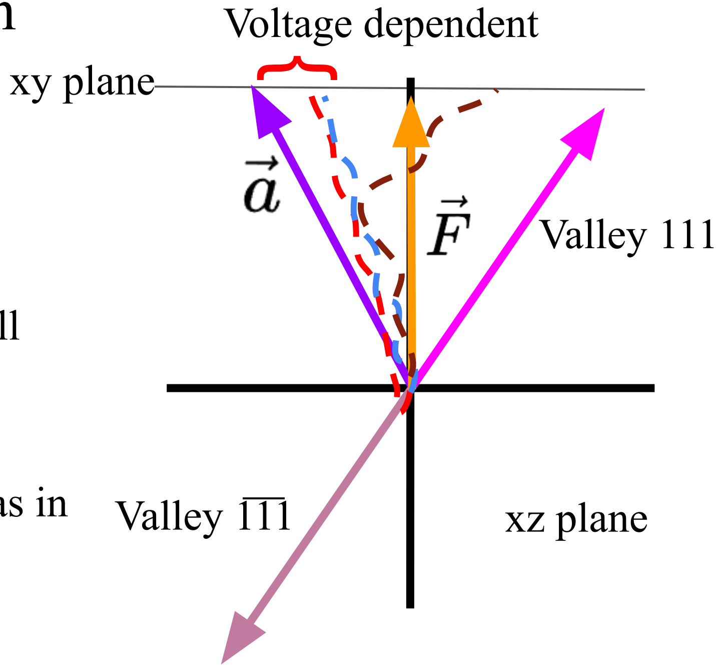
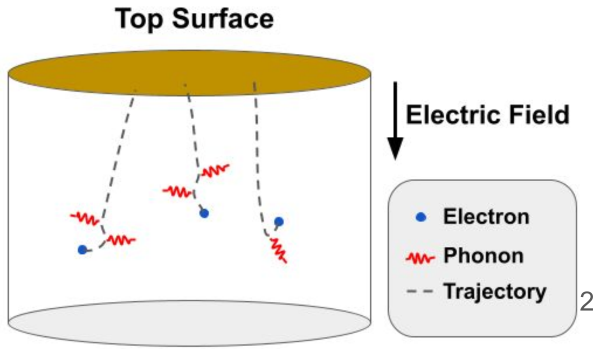
1. Work is in progress on the modeling of interaction rates as functions of charge's energy

Combining effects: Charge Transport Under an Electric Field With Scattering

Incorporating scattering into the electric field modeling, we are left with a qualitative description of the electron trajectories:

- With Intravalley scattering: with a voltage, the trajectories will end up in-between the acceleration direction and the valley direction (blue and red lines)
  - The scattering always pulls them towards the valley (bias in the scattering direction)
  - The voltage always pulls them towards the acceleration direction
- With intervalley scattering: the charge changes its acceleration direction mid-way (brown line)
- The top surface arrival positions depend on both as well as the voltage on the voltage since the electrons always stay low energy due to the intervalley scatterings





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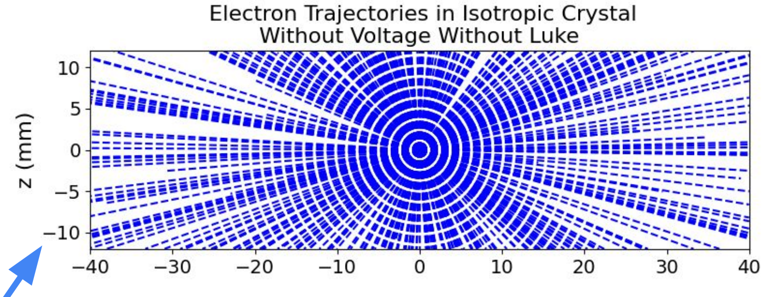
Overview and Goals of a Toy Simulation With Only The Dominant Effects

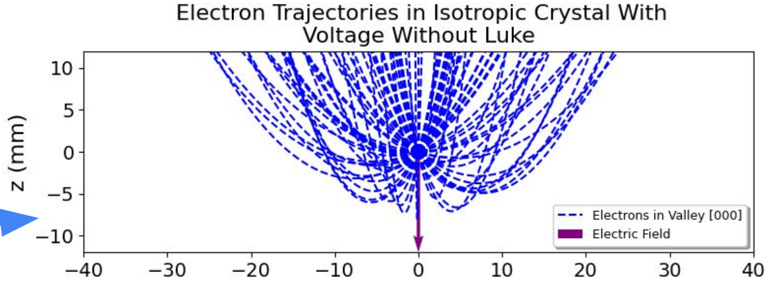
- While our full goal is to have a full Geant4-compatible modeling of charges and phonons, our intermediate goal is to ensure that we understand the expectations from the dominant effects
- In the next slides we present the results of a toy simulation that provides an intuitive sense of how the various effects work together and used for comparisons with the full simulation and, eventually, real data
- We will always follow the same order of adding effects, and highlight the differences between the different crystal structures
- In all cases we have simulated a crystal of 80mm x 80mm x 24mm, all with a monochromatic energy and emanating from the center at x=y=z=0
- The orientation of the silicon crystal is so that the valleys are aligned with the x, y, z axes, while for the germanium case they are aligned with the (±1,±1,±1) directions

Electron Trajectory in an Isotropic Crystal for All Three Effects

Here we show three versions of the trajectories, shown from the side (xz plane), where the voltage is pointing downwards and we consider arrivals on the the top surface (z=12 mm)

- Example trajectories without voltage or scattering:
    - Electrons move in a straight line
- Example trajectories when we add voltage:
    - Electrons gain acceleration in the same direction as the external force
- Example trajectories with Luke scattering added
    - Electrons quickly lose energy and their movement is dominated by the acceleration


Electron Trajectories in Isotropic Crystal Without Voltage Without Luke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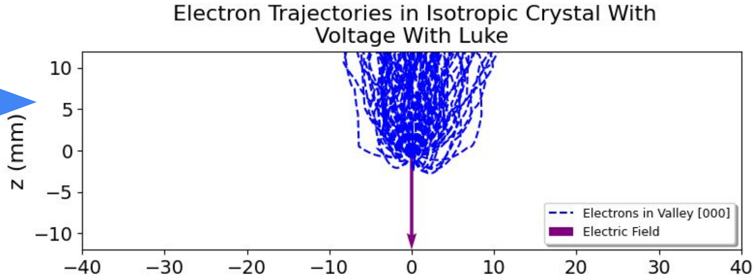
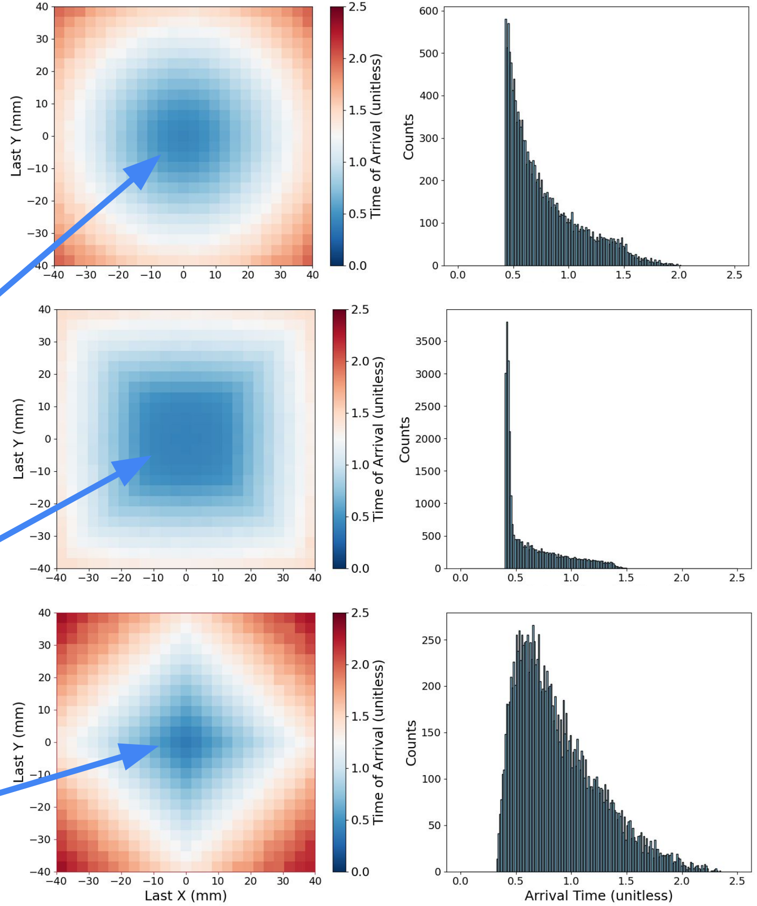

Electron Trajectories in Isotropic Crystal With Voltage With Luke

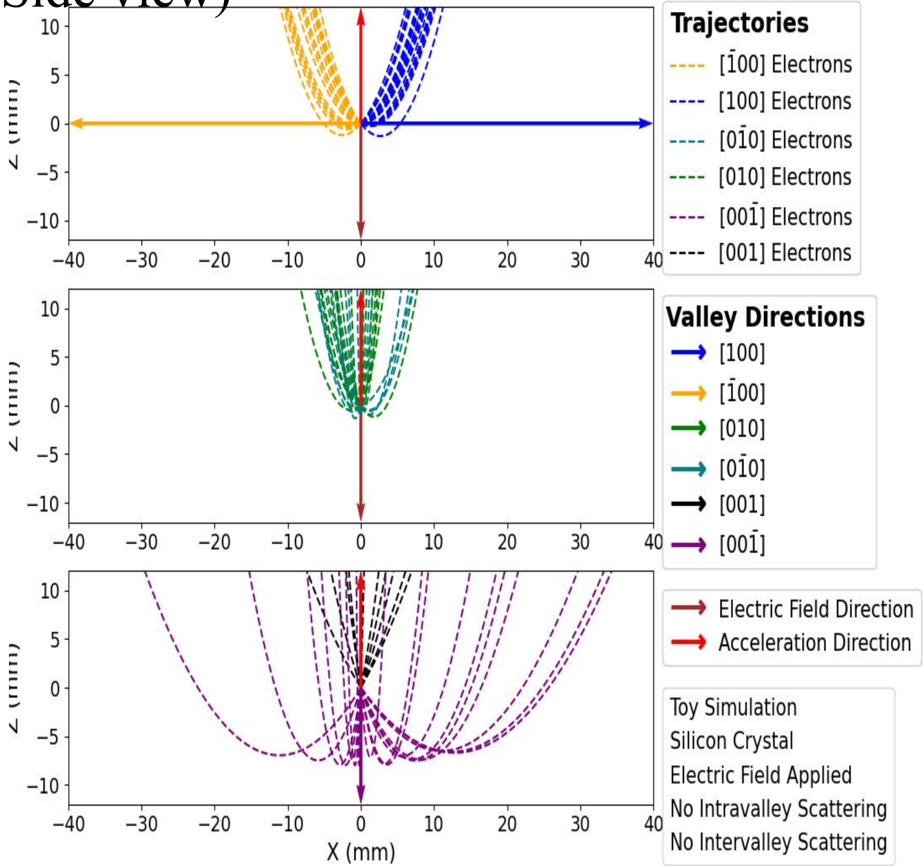
Effect 1: Arrival Time Distributions due to Lattice Valley Effects Only

- Moving to the different crystal types, and focusing on just the arrival times when there is no voltage, we see differences in the speed due to lattice effects
- As there are no voltage, only a portion of the electrons hit the top surface
- Note that the velocity magnitude is less for directions that have less angle with the valleys
    - The isotropic crystal (top plot) has no valleys, so all electrons have the same velocities and the electrons with more angle with z axis arrive later
    - The Silicon crystal (middle plot) has 6 valleys aligned with the x, y, z axes, making the electrons with more angle with z to move faster than the isotropic case
    - The Germanium crystal (bottom plot) has 8 valleys aligned with the (±1,±1,±1) directions making electrons with more angle with z arrive even later



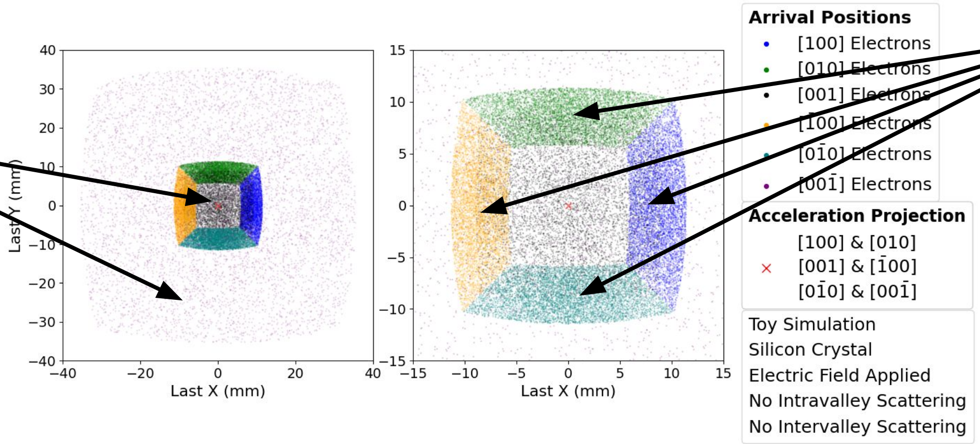
Effect 2: Trajectories in <u>Silicon</u> for Each of the Different Valleys Under an Electric Field <u>Without</u> Scattering Effects (Side view)

- Starting with the silicon case and adding voltage, we separate the trajectories for pairs of valleys
  - Note that these figures are the same as the middle figure for the isotropic case, but in a silicon crystal
- Note that the acceleration for the z axis valleys (third figure) looks smaller than the x and y axes valleys (first and second figures)
- The second plot is basically looking at the first plot from the side



Effect 2: Arrival Positions at the Top Surface in Silicon for Each of the Different Valleys Under an Electric Field Without Scattering Effects (top view)

- Next we combine the results from the six valleys, but consider the arrival position at the top surface (all electrons now reach the top), shown in the left figure (right figure is zoomed in)
- The acceleration direction is the same as the external force as the force is in the same direction or perpendicular to each valley ($a = M^{-1}F$)
- The acceleration magnitude is smaller for the ±z valley (F/m_l) than ±x and ±y valleys (F/m_t), as $m_l > m_t$

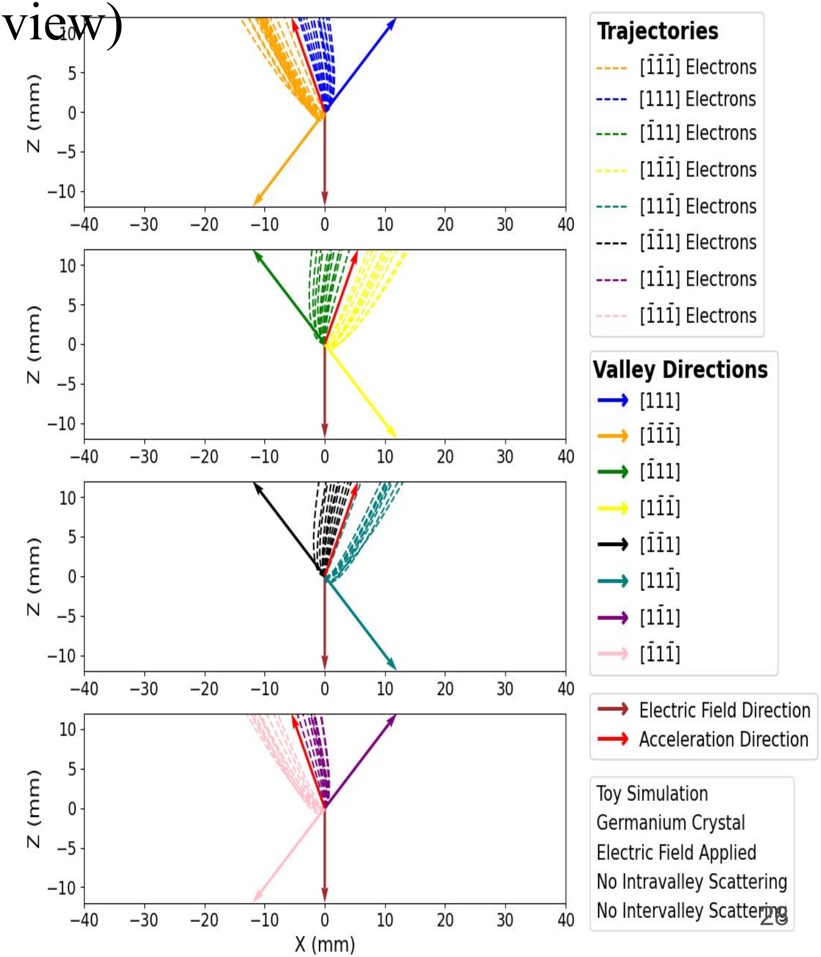


±z valleys electrons (F/m_l)

±x and ±y valleys electrons (F/m_t)

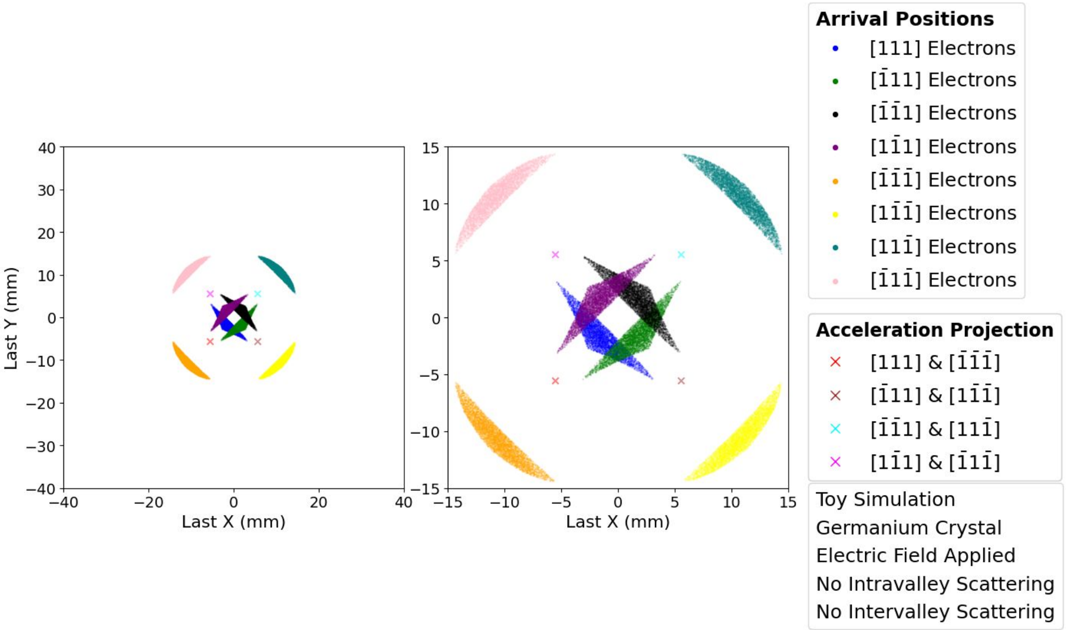
Effect 2: Trajectories in Germanium for Each of the Different Valleys Under an Electric Field Without Scattering Effects (side view)

- Again we show the electron trajectories with a voltage, but with pairs of valleys in a Ge crystal aligned with the (±1,±1,±1) directions
- Note that for all 8 valleys none of the acceleration directions are in the same direction as the external force
- In this special lattice orientation, the valleys all have the same angle relative to the external force
  - The acceleration magnitudes are all identical



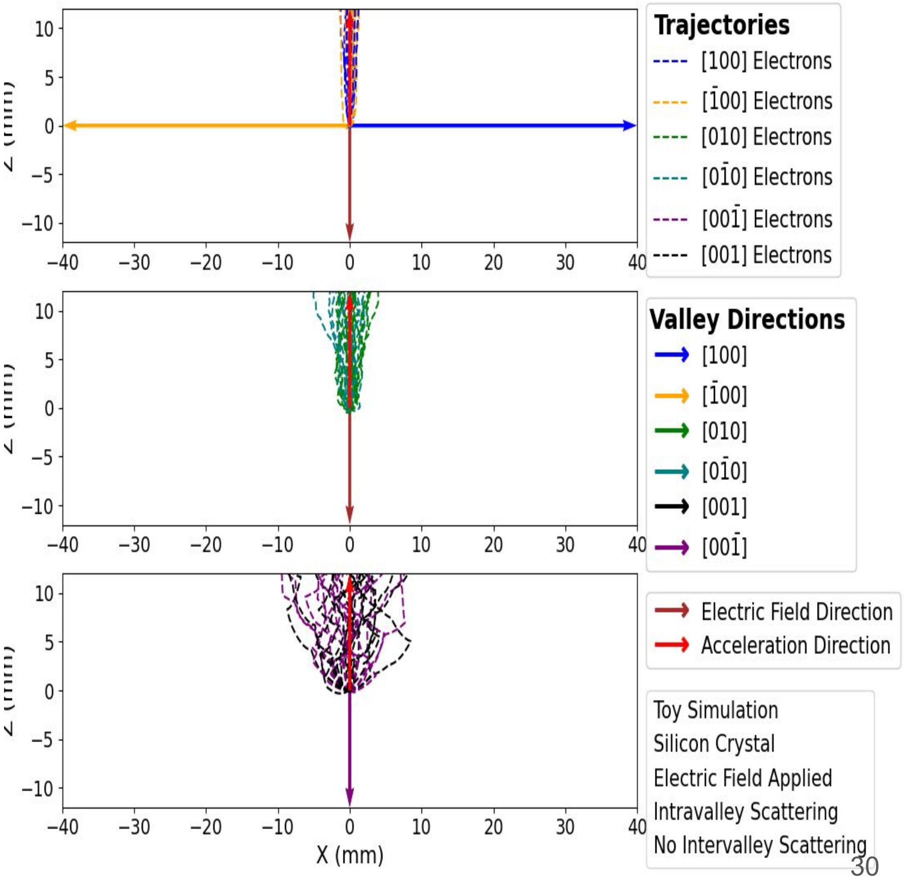
Effect 2: Arrival Positions at the Top Surface in Germanium for Each of the Different Valleys Under an Electric Field Without Scattering Effects (<u>top view</u>)

- Again switching to the arrival positions on the top, we see that the Ge case is less intuitive
- The same energy electrons are divided into 8 groups based on their initial momentum direction (8 octants)
- In the absence of the valleys each octant should make a quadrant in the top surface
- For each valley, the combination of the initial momentum magnitude and the acceleration direction results in 8 separate shapes in the 4 surface quadrants



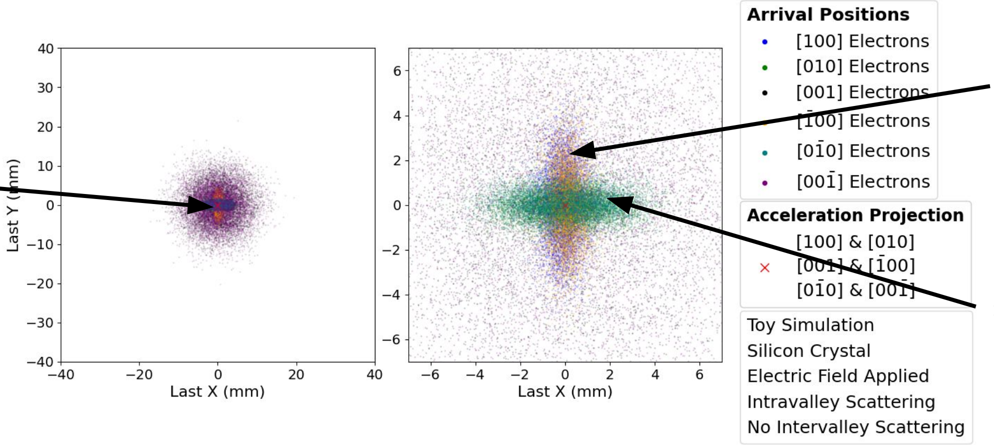
Trajectories in Silicon for Each of the Different Valleys Under an Electric Field With Intravalley Scattering

- Next, we again show the electron trajectories in a silicon crystal, but this time with intravalley (Luke) scattering
- As expected, electrons quickly lose their initial energy and their movement is dominated by the voltage and scattering
- Comparing the first and the second plots you can notice that the electrons with a higher angle with their valley will have higher initial momentum, which means they initially move further perpendicular to the valley



Arrival Positions at the Top Surface in Silicon for Each of the Different Valleys Under an Electric Field With Intravalley Scattering

- Next, looking at the arrival positions on the top, we see a different shape than the no-scattering case for silicon
- Note that the arrival positions are much more focused at the center
- The ±x and ±y valleys electrons arrival position are more spread in ±y and ±x directions, forming a + sign at the middle
- Like the no-scattering case the ±z valleys electrons are much more spread out as they have less acceleration



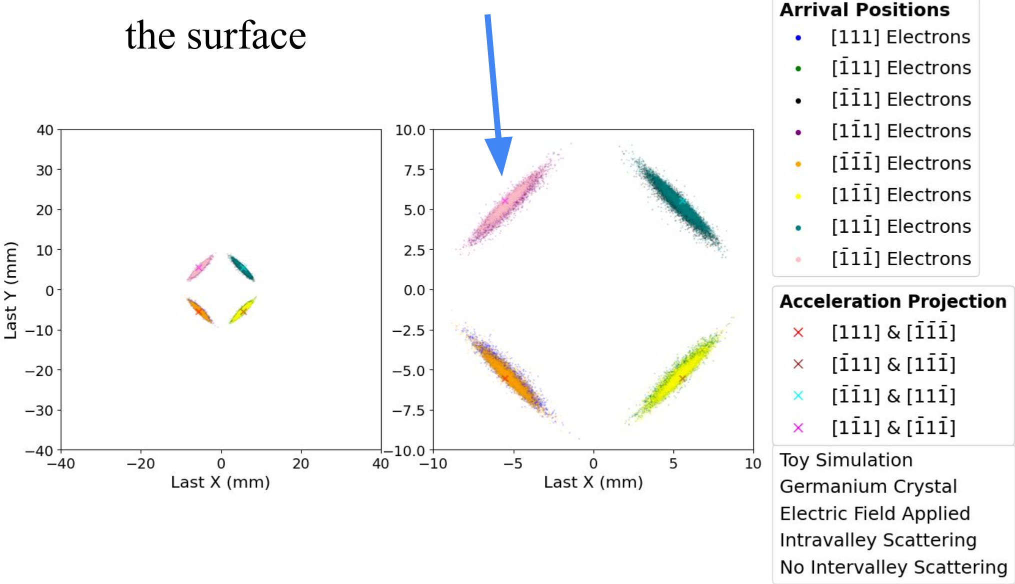
±z valleys electrons

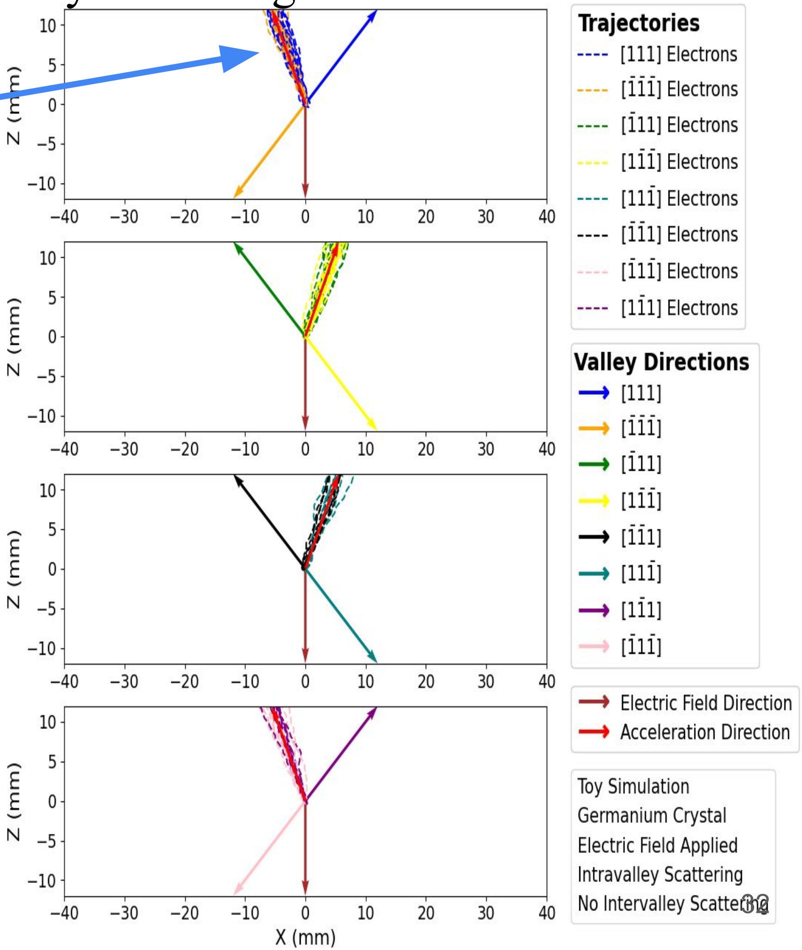
±x valleys electrons

±y valleys electrons

Trajectories and Arrival Positions at the Top Surface in Germanium for Each of the Different Valleys Under an Electric Field With Intravalley Scattering

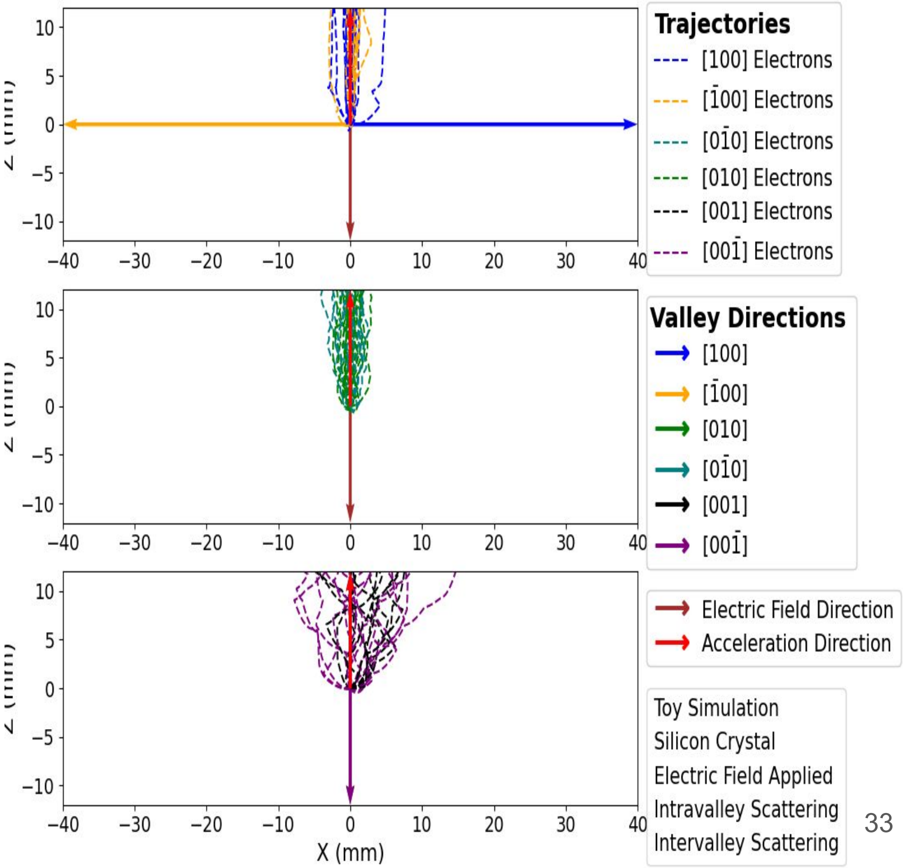
- For the Ge case, the Luke scattering causes all the electrons to quickly lose their initial energy and move along the acceleration direction
- Under strong enough voltage (like we have here) the valley-pair arrival points are essentially merged towards the projection points of the acceleration on the surface





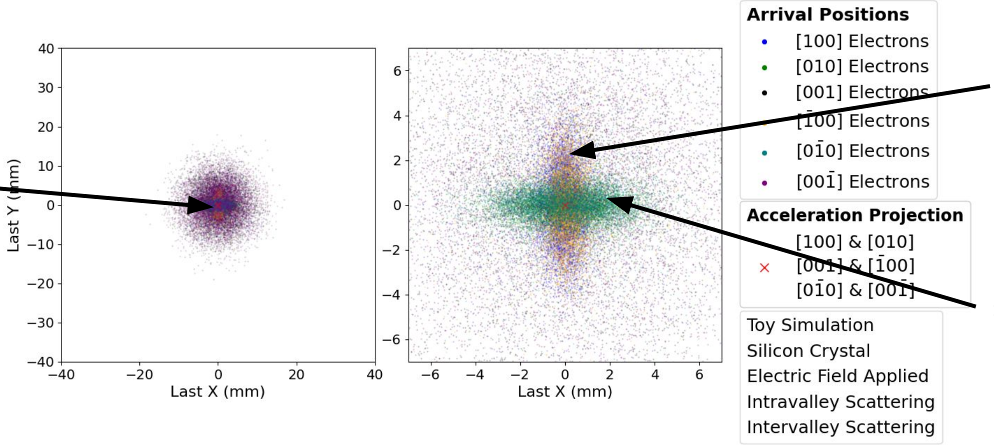
Trajectories in Silicon for Each of the Different Valleys Under an Electric Field With Intravalley and Intervalley Scattering

- Finally, we again show the electron trajectories in a silicon crystal, but this time with both scattering effects
- Electrons now can switch their valleys mid-trajectory
- For the silicon case as all the valleys share the same acceleration direction, only the acceleration magnitude changes, which has minimal impact on the surface arrival positions



Arrival Positions at the Top Surface in Silicon for Each of the Different Valleys Under an Electric Field With Intravalley and Intervalley Scattering

- The arrival positions on the top are not noticeably different
- All electrons share the same acceleration direction
- The different acceleration magnitudes don't affect the arrival position as the intravalley scattering keeps the average velocity low



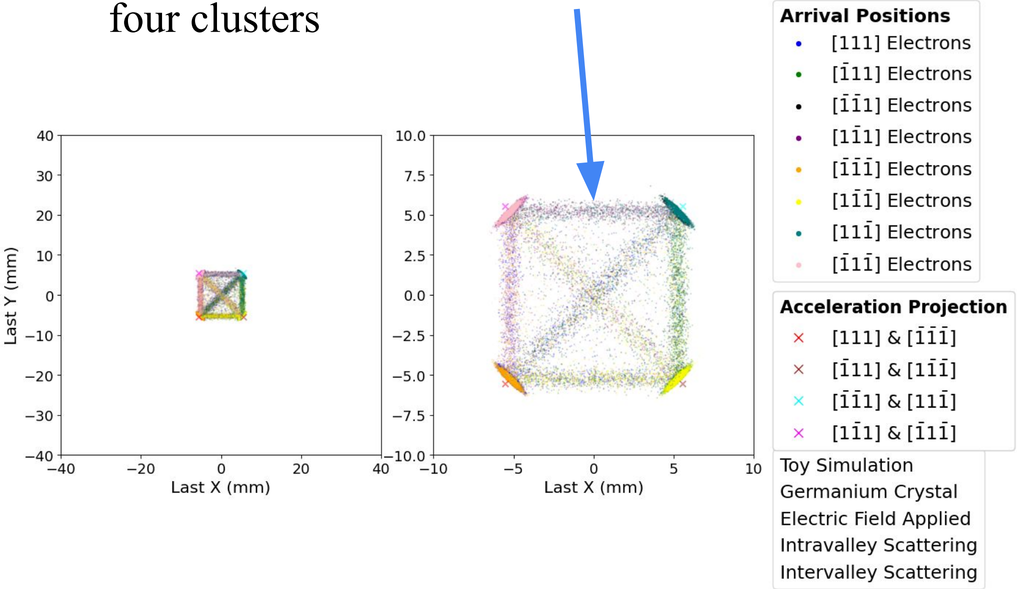
±z valleys electrons

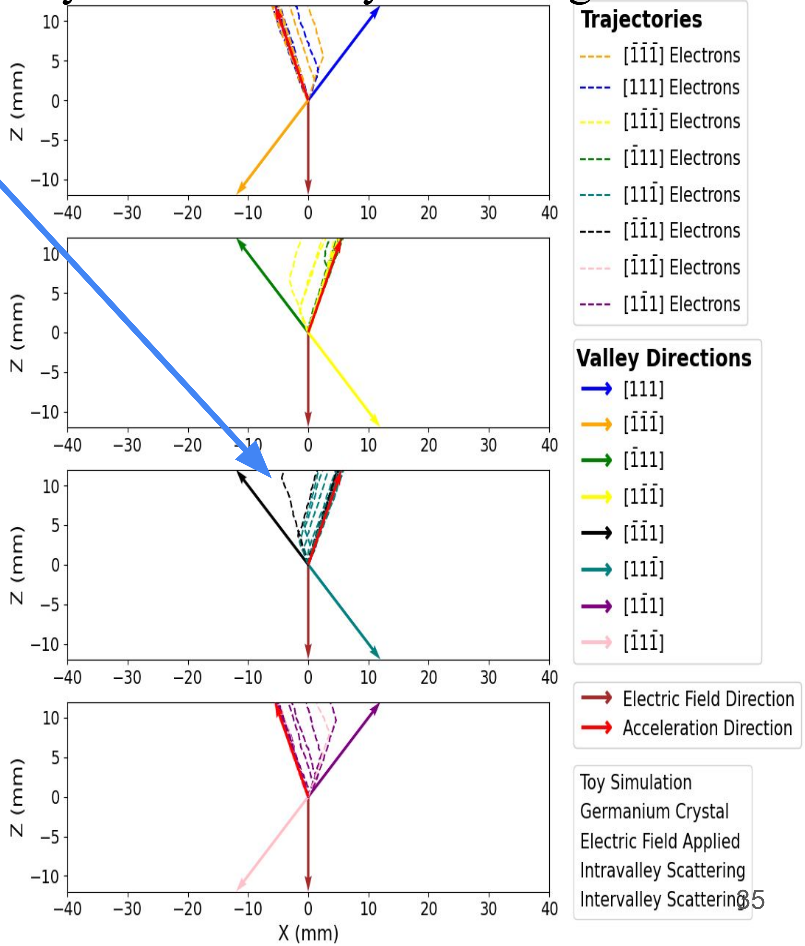
±x valleys electrons

±y valleys electrons

Trajectories and Arrival Positions at the Top Surface in Germanium for Each of the Different Valleys Under an Electric Field With Intravalley and Intervalley Scattering

- For the Ge case, any intervalley scattering causes the electron to get accelerated in different directions mid-trajectory
- This is very noticeable for the Ge case as valleys have different acceleration directions which can cause electrons to end up somewhere between the four clusters





Outline

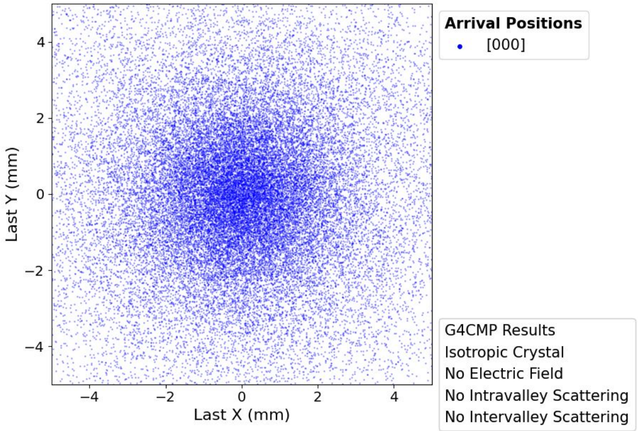
- Introduction and Motivation
  - Dark Matter and Super Cryogenic Dark Matter Search Experiment (SuperCDMS)
  - Charge Arrival Distributions on the Detector Surfaces
  - Thesis Goals
  - SuperCDMS Detector Simulations
- Dominant Effects in the Electron Transportation in a Semiconductor Crystal
  - Energy-Momentum Relationship
  - Electric Field
  - Scattering Effects
- Simulating the Dominant Effects with a Toy Simulation
  - Trajectories
  - Arrival Positions at the Top Surface
- **Geant4 Condensed Matter Physics (G4CMP) Addon**
  - **Overview**
  - **Results and Comparison with Experiment**
- Future Works and Conclusion

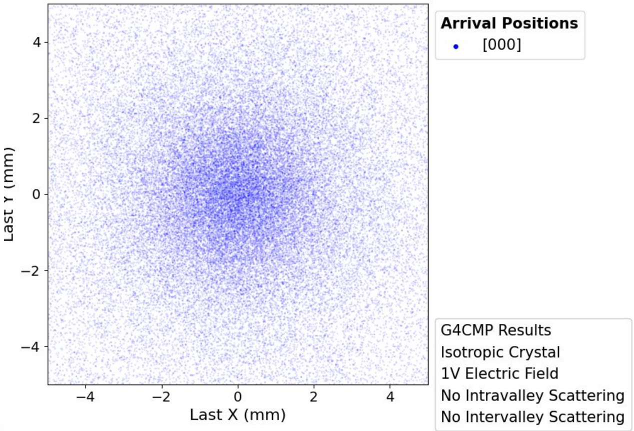
Overview of the Geant4 Condensed Matter Physics (G4CMP) Addon

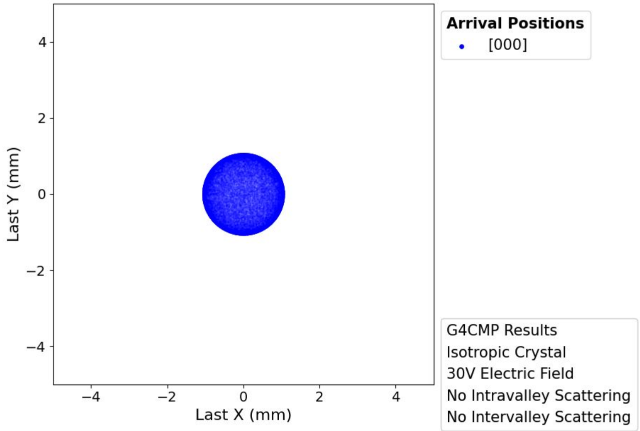
- Since Geant4 does not support anisotropic materials, SuperCDMS uses a custom Geant4 Condensed Matter Physics (G4CMP) addon to make fully quantitative predictions
    - Simulates phonon and charge transport in cryogenic semiconductor crystals using the physics we described earlier
    - Readily incorporates scattering processes and phonon creation
- This add-on allows us to simulate the detector response to both Dark Matter and Standard Model particles. Additionally, there is a wider use for G4CMP in other fields such as study of qbits to increase the accuracy in quantum computing
- When we started this project a number of years ago, G4CMP's charge transportation physics did not reflect the physics discussed in this talk, and in some cases was providing results that did not match our expectations
- Having completed adding all the effects we have described and validating, we next present the comparisons to the toy model, expectations and the data from the testbenches
- To avoid repetition, we note in advance that all the result in next slides match our expectations from the theory and the toy simulation; will show areas of disagreement with real data and needed future work

Electron Arrival Points in an Isotropic Crystal Without Scattering

- These figure shows the density of arrival points at the top surface of a hypothetical square isotropic material with a monoenergetic set of electrons emanating from the center using the full G4CMP simulation with 0V, 1V, and 30V electric field
- By increasing the magnitude of the electric field the electrons focus more around the acceleration direction which aligns with the electric field
- These simplest cases act as a sanity check for G4CMP



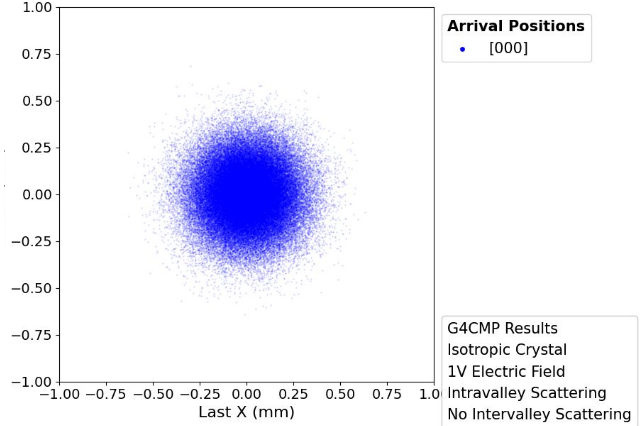


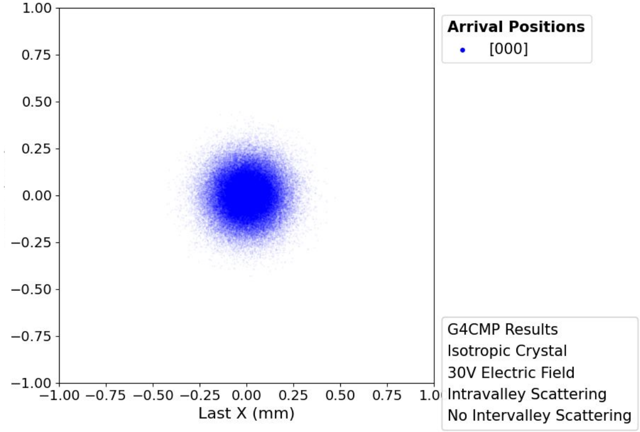


Electron Arrival Points in an Isotropic Crystal <u>With Intravalley</u> Scattering

These results are for the distribution of electron arrival positions on the top surface of an isotropic crystal for 1V and 30V with intravalley scattering. We note:

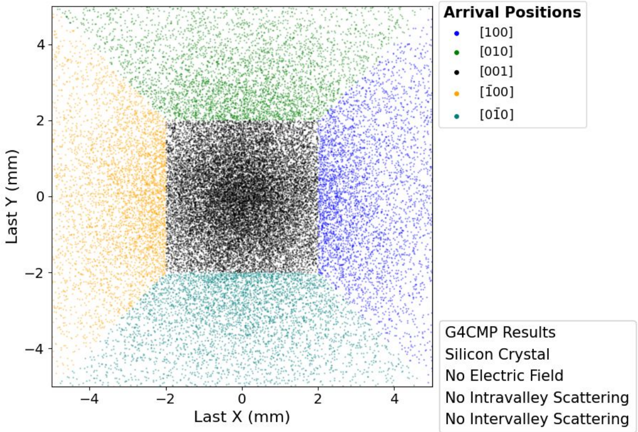
- All electrons now reach the top surface and have results comparable to the high voltage case
- Increasing the voltage has little effect on reducing the cluster size as Luke scattering causes electrons to lose their initial energy rapidly and maintain a relatively constant average speed as the higher energy gain rate leads to a higher frequency of Luke scattering events
- As there are no valleys, we skip the intervalley scattering

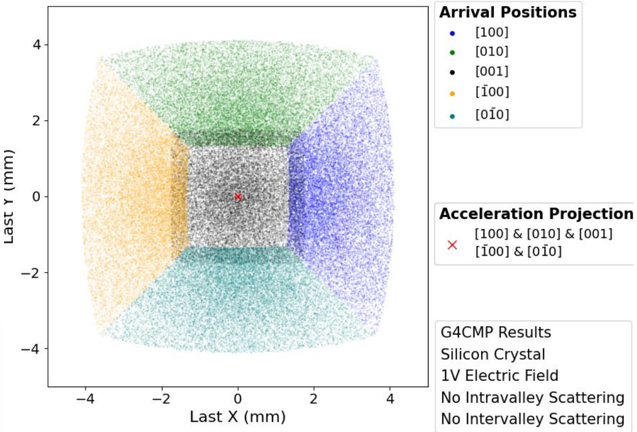


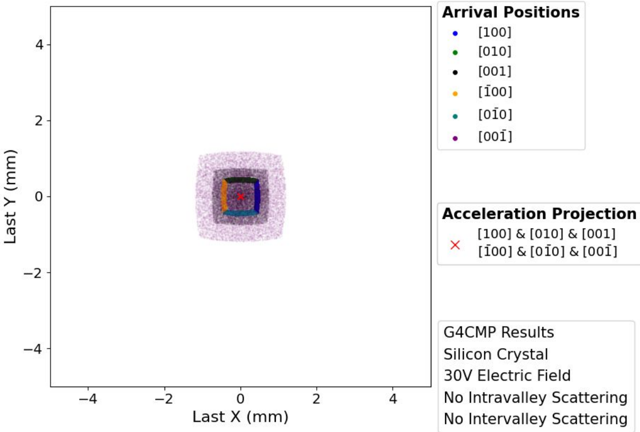


Electron Arrival Points in a Silicon Crystal Without Scattering

- We now move to the first anisotropic case, a Silicon crystal with 0V, 1V, and 30V electric field, without any scattering processes
- By increasing the voltage, acceleration becomes dominant on the electron’s trajectory
- In Si(100), all the electrons in the valleys share the same acceleration direction but experience different acceleration magnitude, resulting in [±100][0±10] valley electrons to get focused towards the center faster than the [00±1] valley electrons

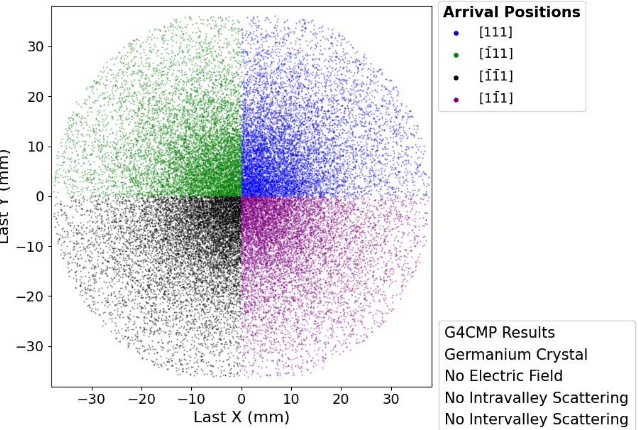


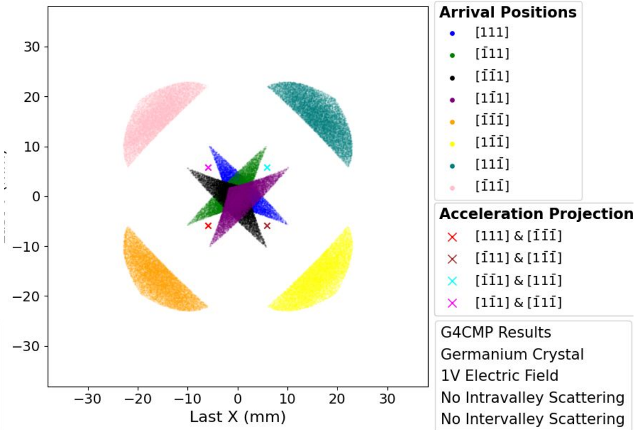


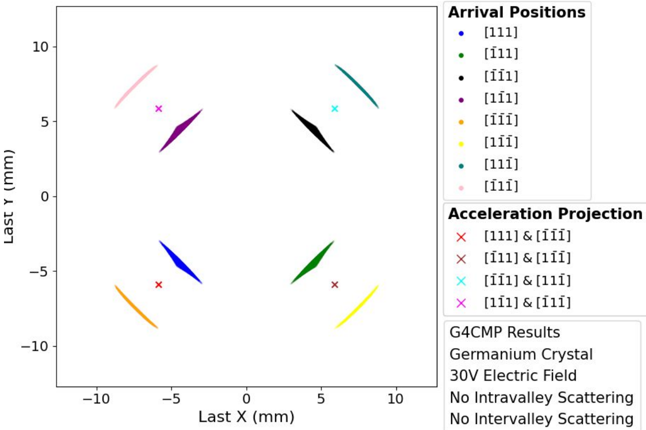


Electron Arrival Points in a Germanium Crystal Without Scattering

- For germanium, all the electrons experience the same acceleration magnitude, but in different directions as shown previously
- We again see that the electrons end up in 8 different clusters, while increasing the voltage decreases the size of each cluster and moves them closer to the acceleration projection points



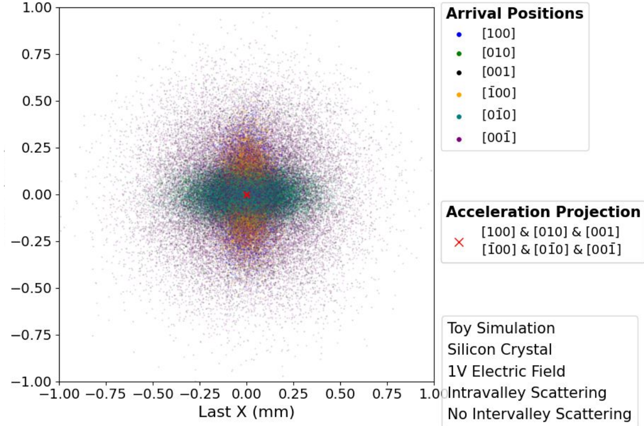


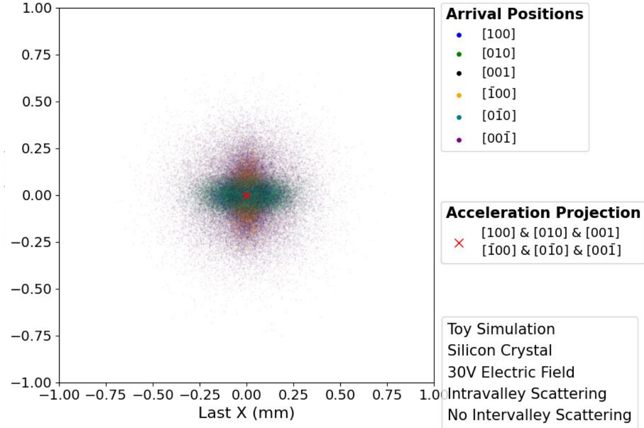


Electron Arrival Points in a <u>Silicon</u> Crystal With <u>Intravalley</u> Scattering

This figure shows the results for the top surface of a silicon crystal with 1V and 30, and intervalley scattering. We note:

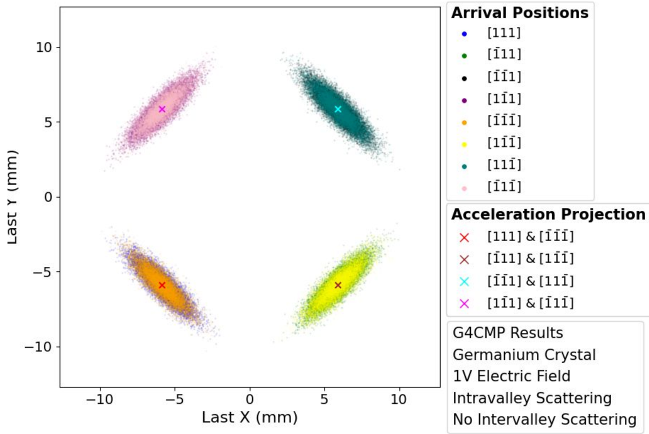
- As expected the electrons are much more focused at the center
- The ±x and ±y valleys electrons arrival position are more spread in ±y and ±x
- The voltage has much less effect on the spread of the arrival positions

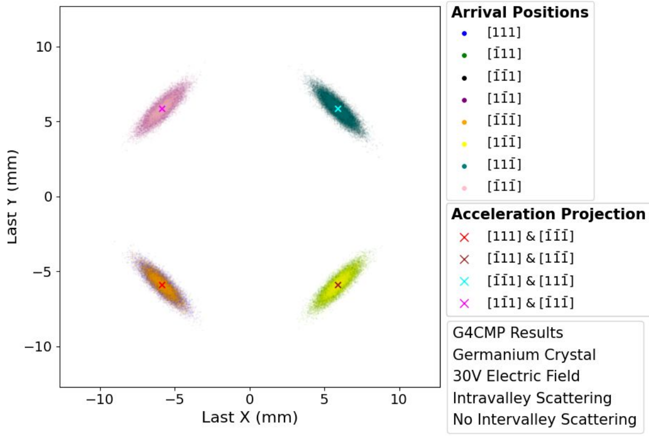




Electron Arrival Points in a Germanium Crystal With Intravalley Scattering

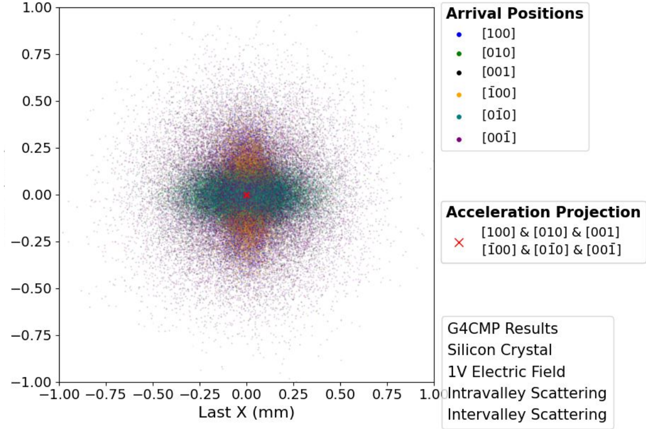
- Moving to the germanium with the same settings, we get the expected 4 clusters instead of 8, forming around the acceleration projection points, essentially combining same-axis valleys as they share acceleration vector
- Again, voltage only slightly reduces the size of each cluster
- We now move to adding the last effect which is intravalley scattering

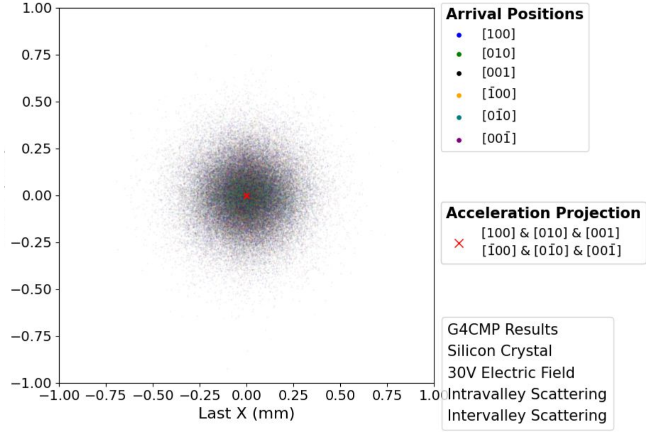




Electron Arrival Points in a Silicon Crystal With All Effects Included

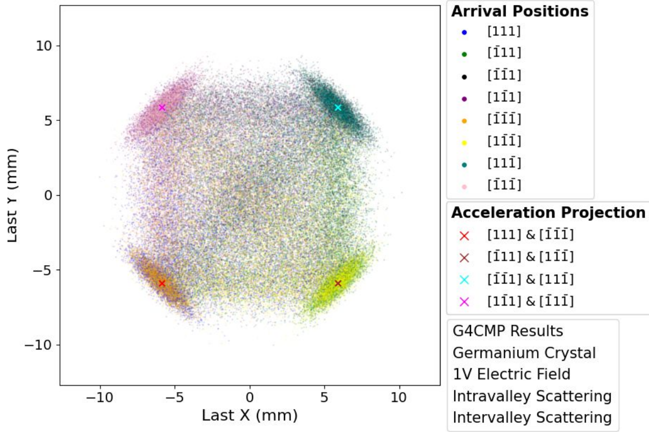
- This figure shows the same setting as before but with intervalley scattering included
- At low voltage the rate of intervalley scattering is too low to have a noticeable impact on the arrival positions
- At high voltage, the intervalley scattering causes electrons to change valleys, effectively mixing the different valley clusters together, which results in the overall shape of the distribution gradually transforming into a circle as the voltage increases

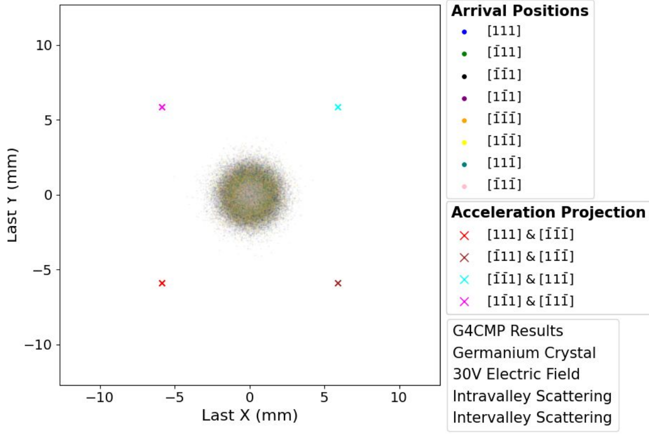




Electron Arrival Points in a Germanium Crystal With All Effects Included

- Lastly, consider the germanium case with all effects included
- In this case intervalley scattering causes some of the electrons to end up between the 4-cluster structure
- Again, we observe that as the intervalley scattering rate increases with voltage, at high enough voltages, the structure is effectively wiped out
- This confirms that all the G4CMP results match our expectations and toy simulation results





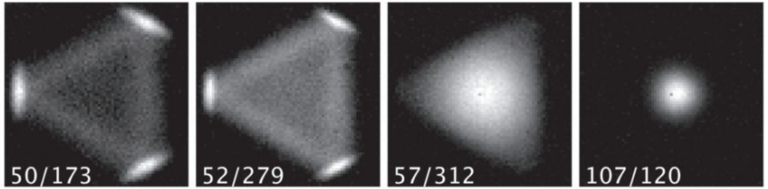
Comparing G4CMP Results with Experimental Results

Experimental configuration differences between G4CMP/SuperCDMS and teststand are non-trivial, but straightforward:

- Lattice orientations
  - Silicon orientation in teststand affects acceleration ==> allows us to see IV scattering effects more clearly
- Temperatures are higher than used in SuperCDMS
  - Parameters that affect trajectories in G4CMP have no temperature dependence

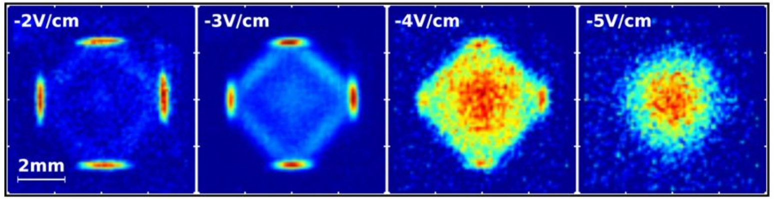
Silicon, 5K temperature, 4 different voltages

Valleys: ±[−1, 0, 1], ±[1, √2, 1] ±[1, −√2, 1]



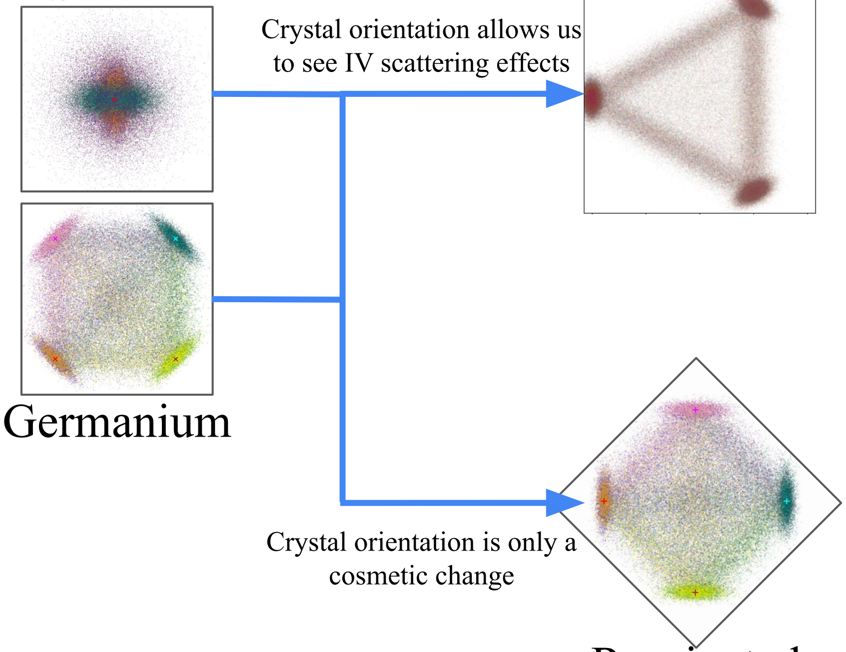
Germanium, 1K temperature, 4 different voltages

Valleys: ±[1, 0, 1], ±[−1, 0, 1] ±[0, 1, 1], and ±[0, -1, 1]



Comparing G4CMP Results with Experimental Results

1. For the silicon case, previously, all the acceleration vectors had the same direction but different magnitude, but now they have the same magnitude but different directions, resulting in a triangular shape (same as the germanium case, but with 3 clusters instead of 4, resulting in a triangle instead of a square)
2. The germanium case is directly comparable to the results presented in previous slides, but with a simple rotation



Silicon

Germanium

Reoriented Silicon

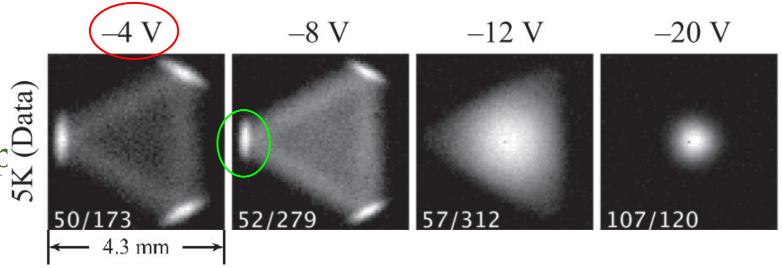
Crystal orientation allows us to see IV scattering effects

Reoriented Germanium

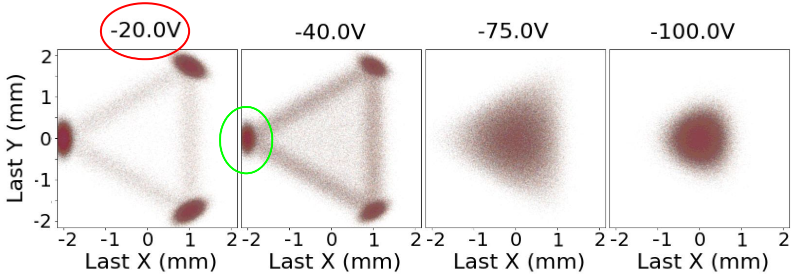
Crystal orientation is only a cosmetic change

Comparison With Experiment - Silicon

- We see qualitative agreement, but quantitative disagreement between experimental and G4CMP results
  - The positions of the electrons that did not go through any intervalley scatterings (the triangle vertices) look the same, independent of the voltage and temperature
  - The arrival distributions and their evolution with voltage qualitatively match the experiment (as the voltage goes up we see the triangle filling in more)
  - G4CMP results seem to mimic the experimental results, but at much higher voltages
- This suggests that the quantitative disagreement arises from the values of the intervalley scattering rate parameters
  - We note that those parameters were tuned with an older version of G4CMP, prior to our changes
  - For quantitative predictions carefully re-calibrated intervalley scattering rates will be necessary



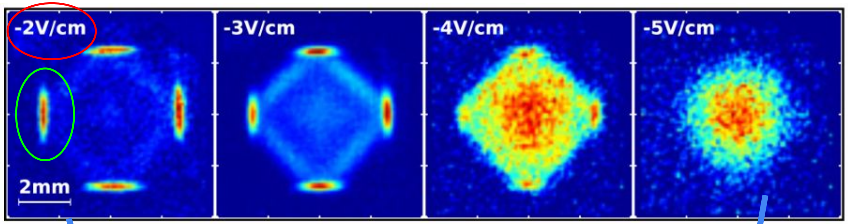
Si Experimental Results



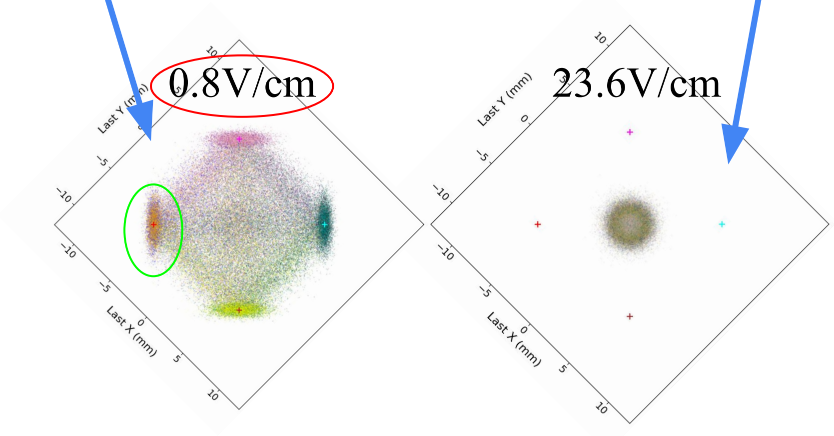
Si G4CMP Results

Comparison With Experiment - Germanium

- We again see qualitative agreement, but quantitative disagreement:
  - Different crystal sizes and electron path lengths result in different spot positions for the corners, but they agree after simple scaling and rotation
  - As with silicon, the experimental data for electron arrivals between the clusters show the same trends as a function of voltage but different values where it happens
- Again this suggests the need for improvement in the intervalley scattering rate calculations



Ge Experimental Results



Ge G4CMP Results
Rotated by 45 Degrees

Future Work

While the G4CMP results show excellent qualitative agreement with data, future work will be necessary to get quantitative agreement. We note two ongoing parallel efforts:

- Since the current parameters for intervalley scattering rates were determined using an older version of G4CMP, before these changes, resulting in incorrect rates, a re-tuning campaign is in progress for both crystal types
- Since the intervalley rates are modeled as a function of voltage instead of charge energy, there is a program of work to develop a new intervalley scattering model based on charge energy using first principles
  - Such intervalley scattering model can also eliminate the need of tuning intervalley scattering rate parameters for every new crystal

Conclusions

- We have described the modeling of the dominant charge transport effects in single-crystal detectors and implemented them in the G4CMP software package
- We have provided intuitive ways of understanding the expectations in various scenarios for each of the various combinations, and confirmed that the simulations qualitatively match both our expectations and the experimental results
- While a comprehensive quantitative comparison will require future work on the intervalley scattering rates, we expect this powerful tool to be used in the analysis of the upcoming data taking run at SNOLAB as well as quantum computing devices
    - With luck, it may be the needed piece that helps us get to a major discovery

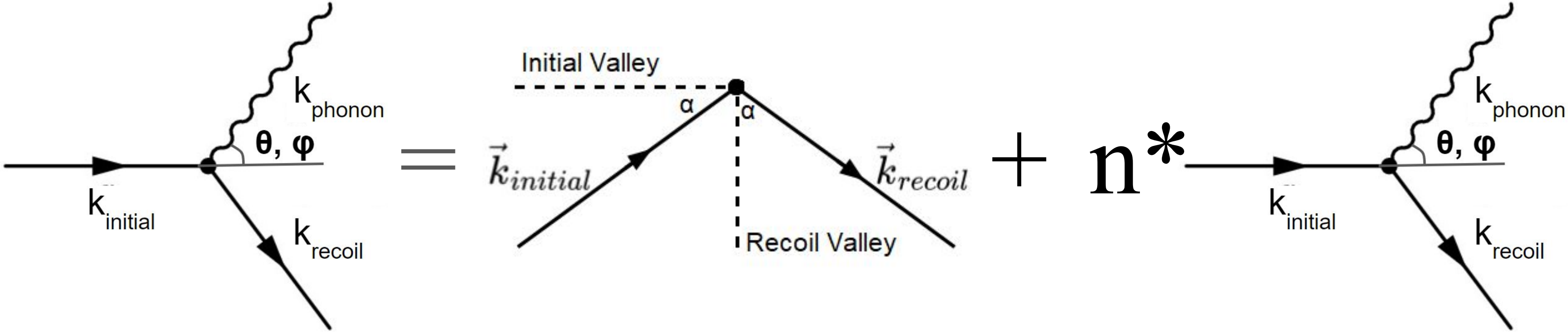
Thank You

Backup Slides

Scattering in a Semiconductor Crystal (Modeling)

In an optical phonon scattering in macroscopic view:

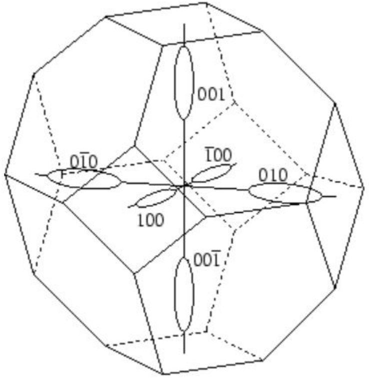
- The phonon would quickly downconvert, the final state would essentially be an electron in a different valley and multiple low-energy phonons
- It is indistinguishable from the combination of a neutral impurity scattering and multiple acoustic phonon scatterings



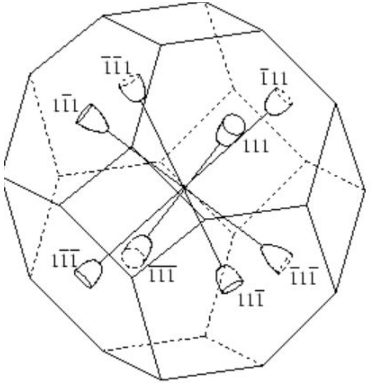
Optical Phonon Emission   Elastic Intervalley Scattering   Acoustic Phonon Emission

L and X directions in the Brillouin Zone

- These figures show a three diagrams which illustrate the periodic structure of a crystal in the reciprocal lattice of a face-centered cubic (FCC) structure
- Important points in the Brillouin zone of an FCC lattice include the X points at the centers of square faces (top diagram) and the L points at the centers of hexagonal faces (bottom diagram) in which the energy of an electron in conduction band will be minimized
- It turns out that the X points will be the “valleys” directions for silicon and the L points will be the “valleys” directions for germanium



X directions in Brillouin Zone



L directions in Brillouin Zone

Band Gaps for Si and Ge in SuperCDMS Settings

- For Silicon the the lowest conduction band energy level is for charges with a wavevector along the six X directions in the Brillouin Zone and this band gap is equal to:

$$E_g = 0.7437 - \frac{4.77\times10^{-4}T^2}{T+235}\ \text{eV}$$

- For Germanium the the lowest conduction band energy level is for charges with a wavevector along the eight L directions in the Brillouin Zone and this band gap is equal to:

$$E_g = 1.166 - \frac{4.73\times10^{-4}T^2}{T+636}\ \text{eV}$$

- SuperCDMS detectors work at around 50mK temperature, which means a band gap of **<u>1.116eV</u>** for Silicon and a bang gap of **<u>0.7437eV</u>** for Germanium