Modeling Hole Transport on the Surface of Ge Gamma-Ray Detectors

Nuclear Physics SBIR/STTR Exchange Meeting, September 13-14, 2010

Presented by: Cory Ahrens PI: Paul Mullowney
Kevin Paul, Ming-Chieh Lin, Michael Loh (Tech-X Corp)
David Radford, Ren Cooper, Karen Lagergren (ORNL)
ahrens@txcorp.com/paulm@txcorp.com

Tech-X Corporation
5621 Arapahoe Ave., Boulder, CO 80303
http://www.txcorp.com

This work was supported by
DOE SBIR Phase II Award No. DE-FG02-07ER84758
Office of Nuclear Physics

TECH-X CORPORATION

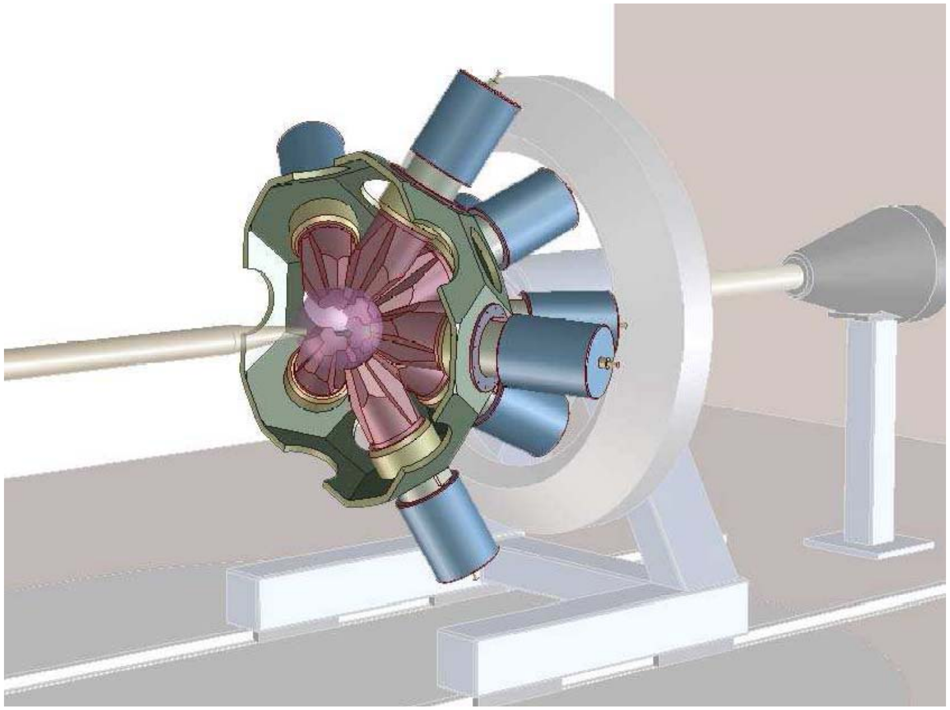
Outline

- Background
- Phase II objectives
- Work so far and results
- Conclusions
- Current and future work

GRETINA

GRETINA=Gamma Ray Energy TrackINg Array

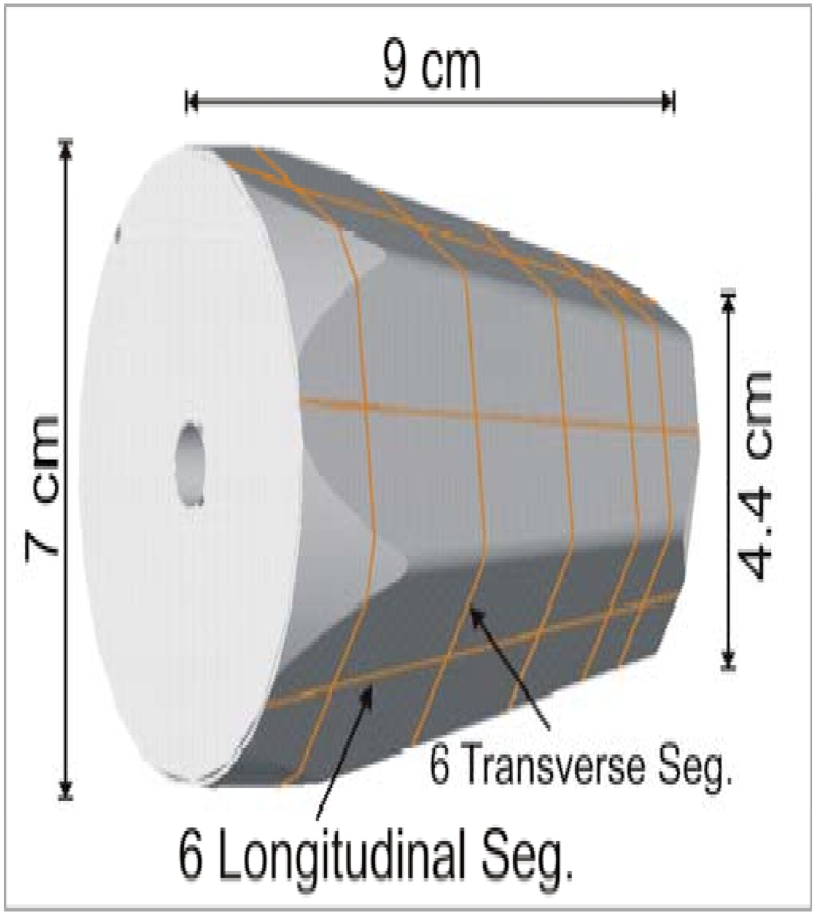
- Used for in-beam nuclear structure studies
- 28 segmented HPGe detectors
- ~ 1π steradians
- 3D position sensitive (~1mm) detector
- Completion in 2011
- Predecessor to GRETA



TECH-X CORPORATION

Segmented GRETINA Detector

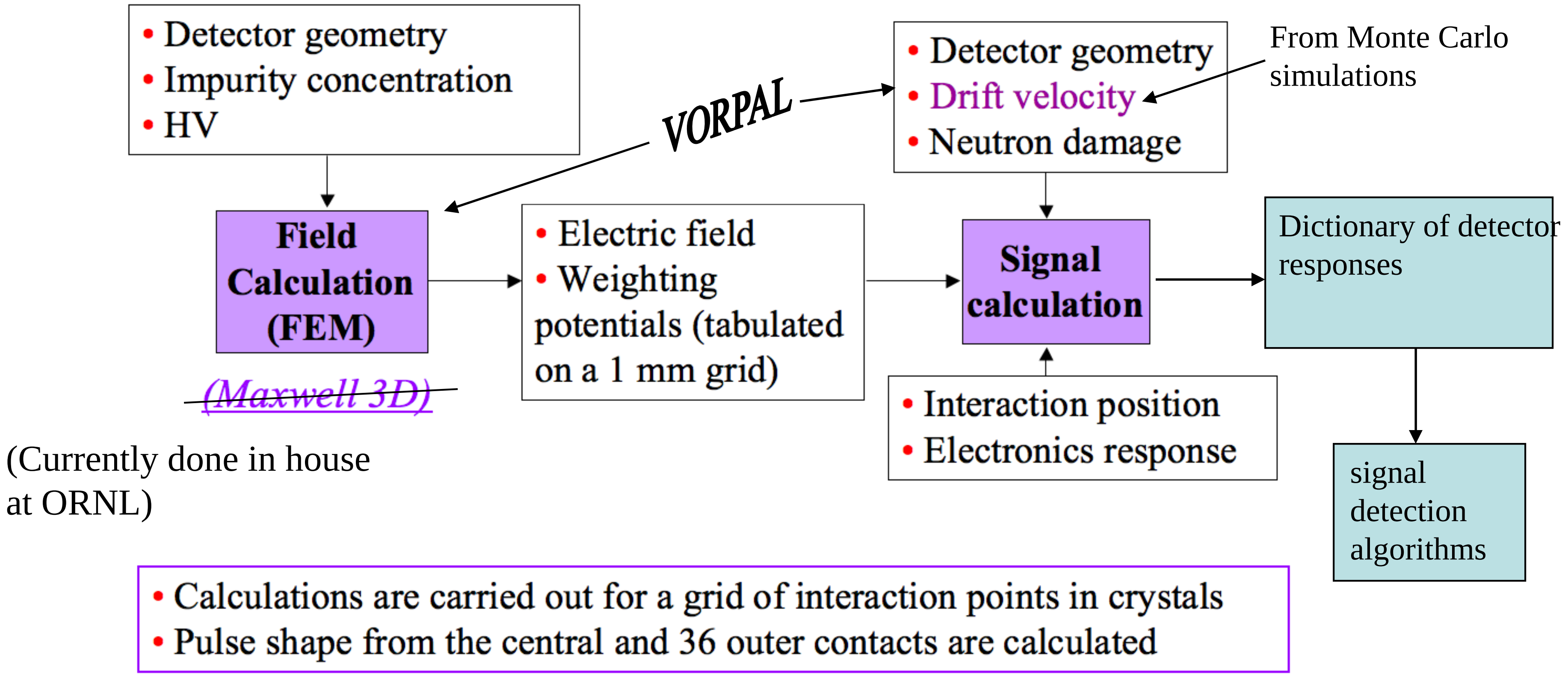
High spatial resolution of γ-ray interactions



- Detector composed of 36-fold segmented Germanium crystals.
- Incoming gamma rays create electron/hole pairs via Compton scattering.

- In crystal bulk, simple valence band models yield highly accurate values for hole drift/diffusion coefficients (~1-2% error)
- Behavior along surfaces is highly pathological.

GRETINA Modeling Framework



- Detector geometry
- Impurity concentration
- HV

VORPAL

- Detector geometry
- Drift velocity
- Neutron damage

From Monte Carlo simulations

Field Calculation (FEM)

~~(Maxwell 3D)~~

(Currently done in house at ORNL)

- Electric field
- Weighting potentials (tabulated on a 1 mm grid)

Signal calculation

- Interaction position
- Electronics response

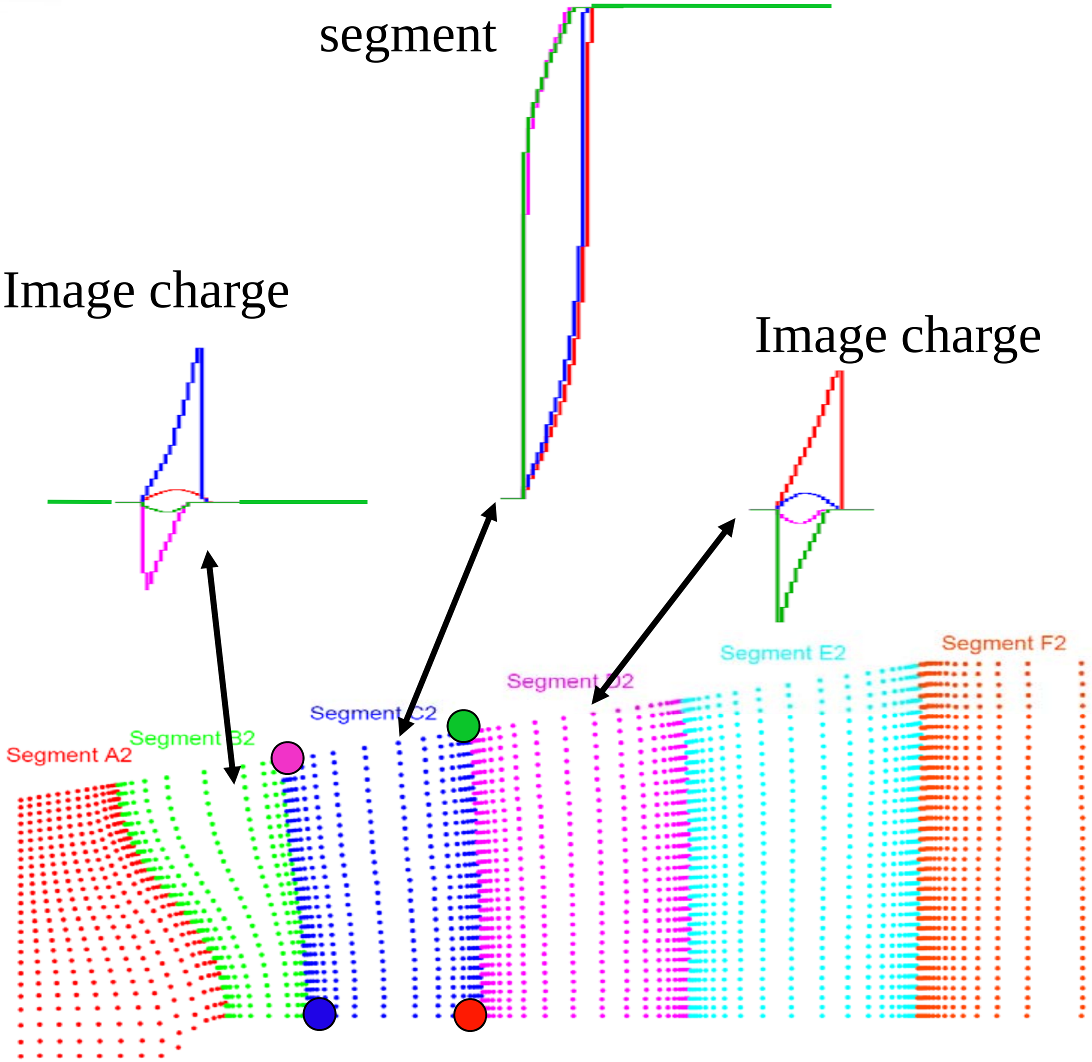
Dictionary of detector responses

signal detection algorithms

- Calculations are carried out for a grid of interaction points in crystals
- Pulse shape from the central and 36 outer contacts are calculated

Current modeling effort : encapsulate this infrastructure within VORPAL

Calculated signals: sensitivity to position



Hit segment

Image charge

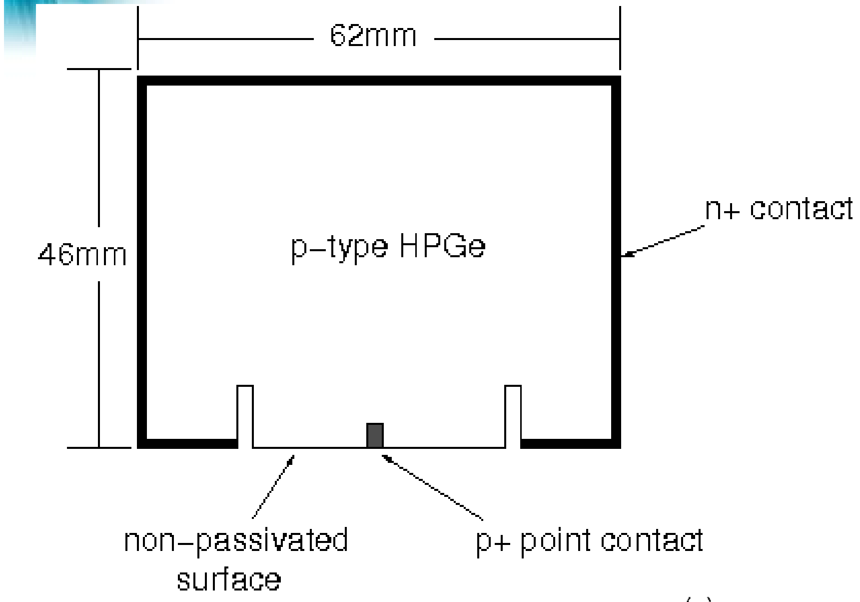
Image charge

Signals color-coded for position

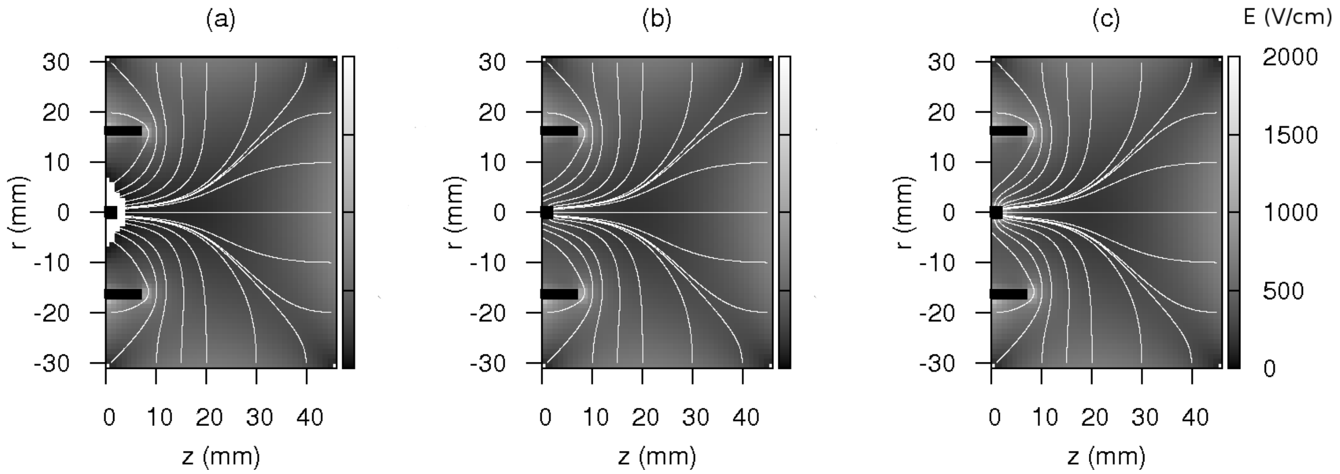
Signals are nonlinear with respect to position; necessary to extract multiple positions.

Pathological Surface Signals

Consider a simpler Germanium PPC detector

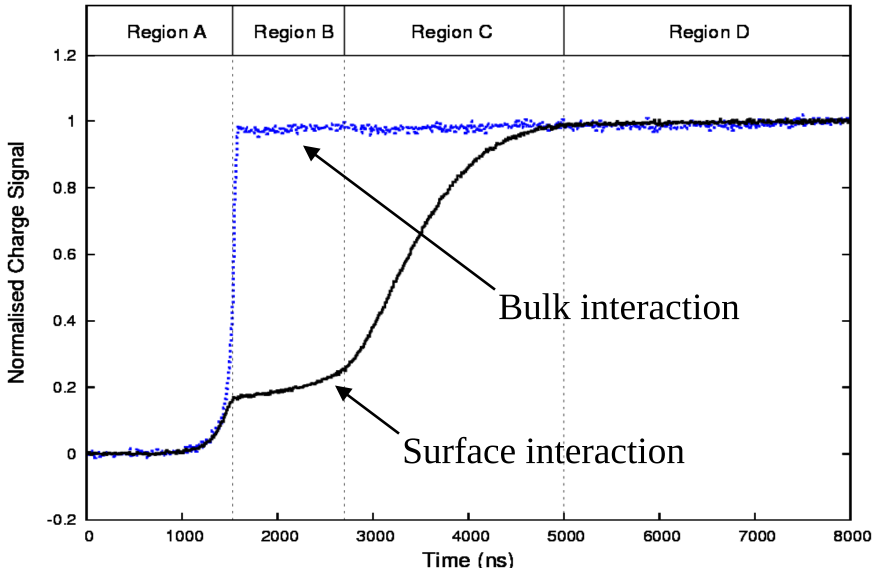


Fields calculated with spatially uniform negative surface charge distribution on non-passivated face. Overlaid are hole trajectories associated with a range of interaction positions. Calculations of the electric field within the PPC detector at (a) 300 V below depletion, (b) depletion and (c) 200 V above depletion.



Manufactured by PHDs Co.

Pathological Surface Signals (continued)



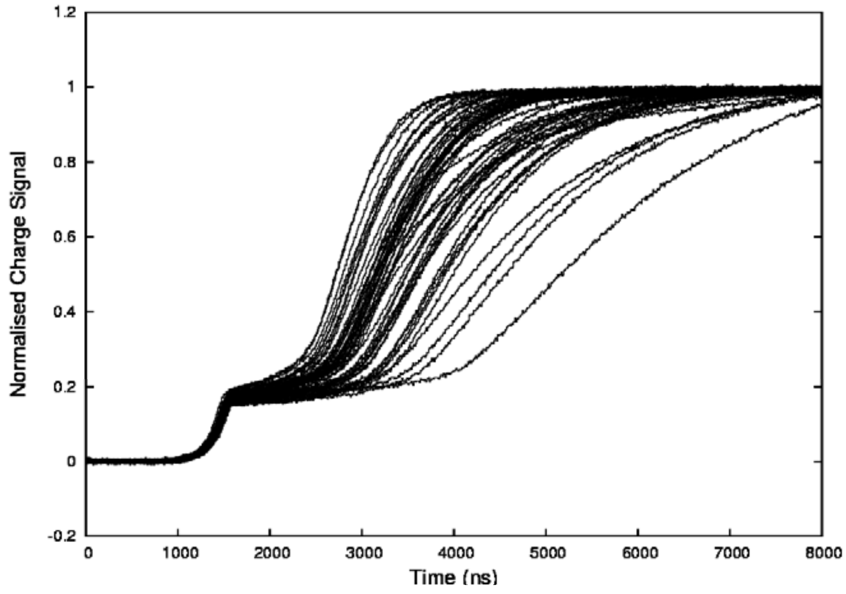
Bulk interaction

Surface interaction

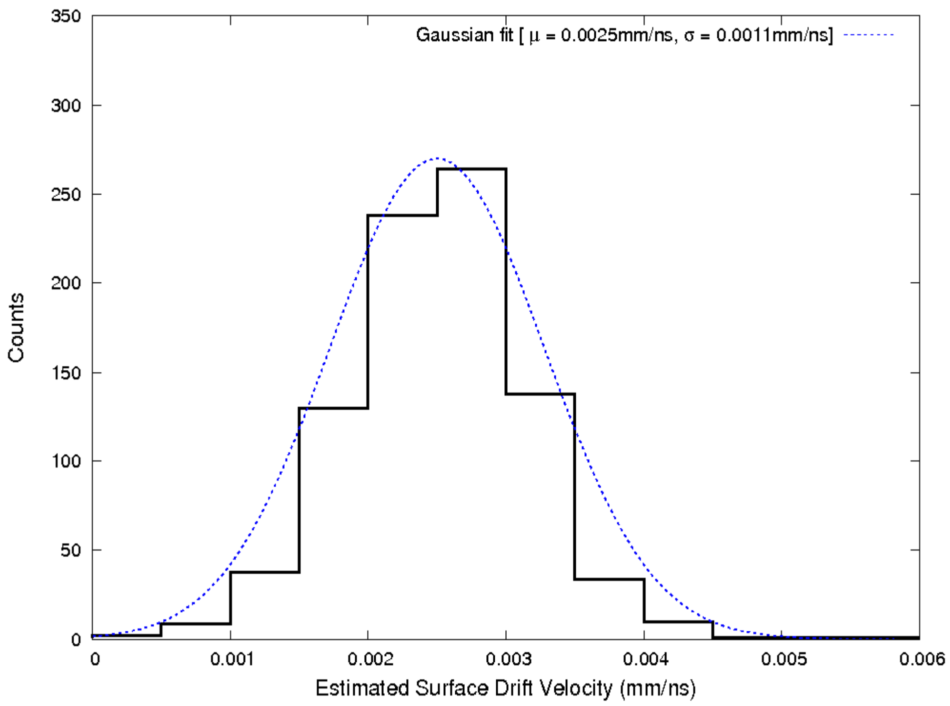
- A : Normal Bulk Charge motion
- B : Plateau for ~500 ns
- C : Acceleration (still impaired motion)
- D : Pulse reaches a maximum

Example of anomalous signal recorded when PPC detector was operated close to depletion.

Regions of the pulse shape have been highlighted to show the key features. For comparison, a signal representing the typical response of the PPC detector is overlaid (dashed blue line).



Surface Drift Velocity Estimation



- Histogram of radial drift velocity estimated from one thousand anomalous events.

- Guassian fit to the data yields a mean value of 0.0025 (±0.0011) mm/ns, or 2500 m/s

- A factor of 40 slower than the accepted value for hole drift in bulk HPGe

- Means timing characteristics of interactions near surface MUCH different than those in the bulk

- Need to model/understand near surface transport

Phase II Project Objectives

We have three technical objectives in the Phase II project whose feasibility has been demonstrated in the Phase I project.

Objective 1: Demonstrate the ability to accurately model carrier mobility in the crystal bulk. (Done—will show results)

Objective 2: Demonstrate the ability to accurately compute the electric field around the passivated surface. (currently at ORNL, moving to VORPAL)

Objective 3: Develop a more accurate determination of the gamma ray event location near the non-passivated surface. (Rest of this talk)

Valence Band Structure for Monte Carlo Simulations

- Band structure incorporated in dispersion relation:
- Determines energy vs. velocity and group velocity for MC simulations
- Analytic models (Warped, Parabolic, Elliptic, etc.)
  - Straight forward to compute scattering probabilities between crystal and particle
  - Can include binary interactions: carrier-carrier scattering in a straightforward manner
  - Models have small range of validity in energy domain around the band maxima (valence) or minima (conduction)
- Numerical models (e.g., k.p and full band)
  - Wider range of validity in energy domain
  - Scattering probabilities are far more computationally intensive
- Numerical models may be necessary on surfaces where band structure is complicated, e.g., sub-band splitting due to surface electronic structure (confinement), surface E-fields, 2D DOS, etc.

Warped Band Model (3D)

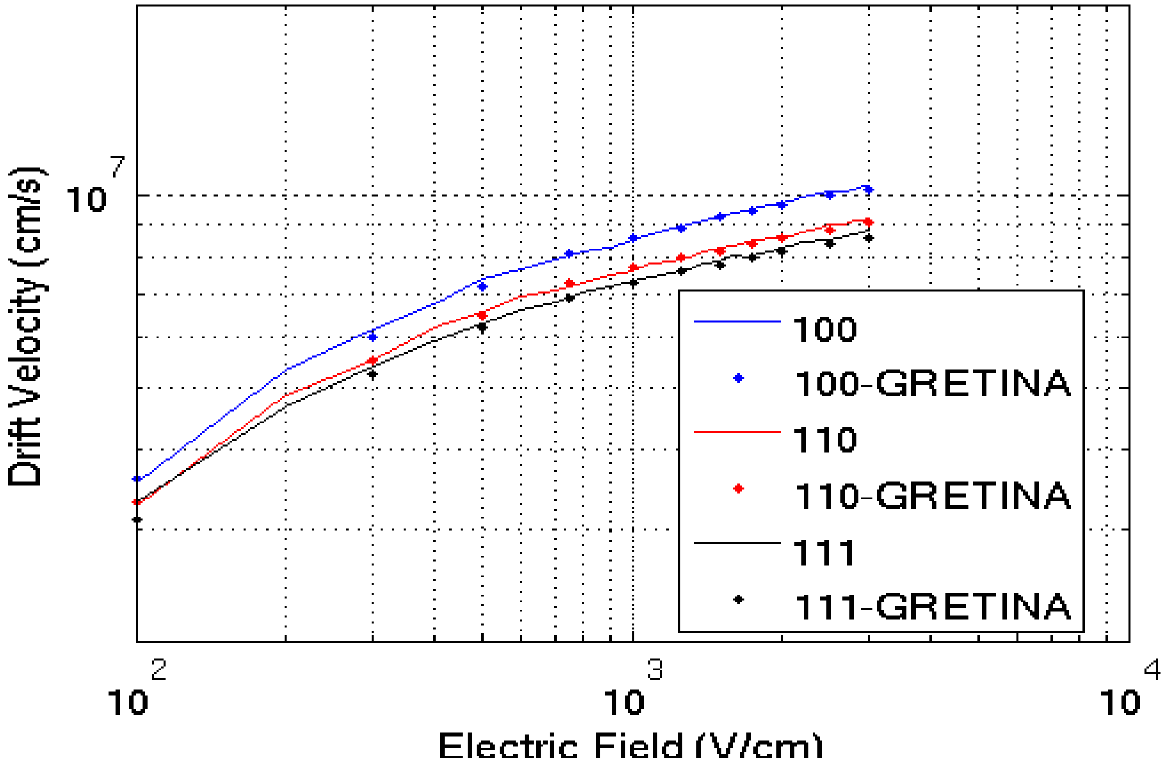
- Classical simple model of the heavy/light hole

$$\epsilon(\mathbf{k}) = \frac{\hbar^2|A|}{2m}k^2[1 \mp g(\theta,\psi)]$$

- Model calculations depends on crystal properties, e.g., material speed of sound, temperature, density, etc.
- Cyclotron resonance experiments are used to determine band parameters.
- Density of states calculations shows that heavy hole has ~95% occupation, the light hole has ~5% occupation, and the spin orbit has ~0.01% occupation
- For high field setting, can improve results by considering interband transitions and including non-parapolic effects

Warped Band Model (cont.)

- Using a single heavy hole (including non-parabolicity) can yield highly accurate values for the bulk drift velocity.



- Model can also give accurate computations of hole transverse and longitudinal diffusion

Surface Valence Band Models

- Very hard to calculate the valence band structure accurately in surface inversion layers
- Couple Schrodinger and Poisson (in surface normal direction) in order to get dispersion relation:

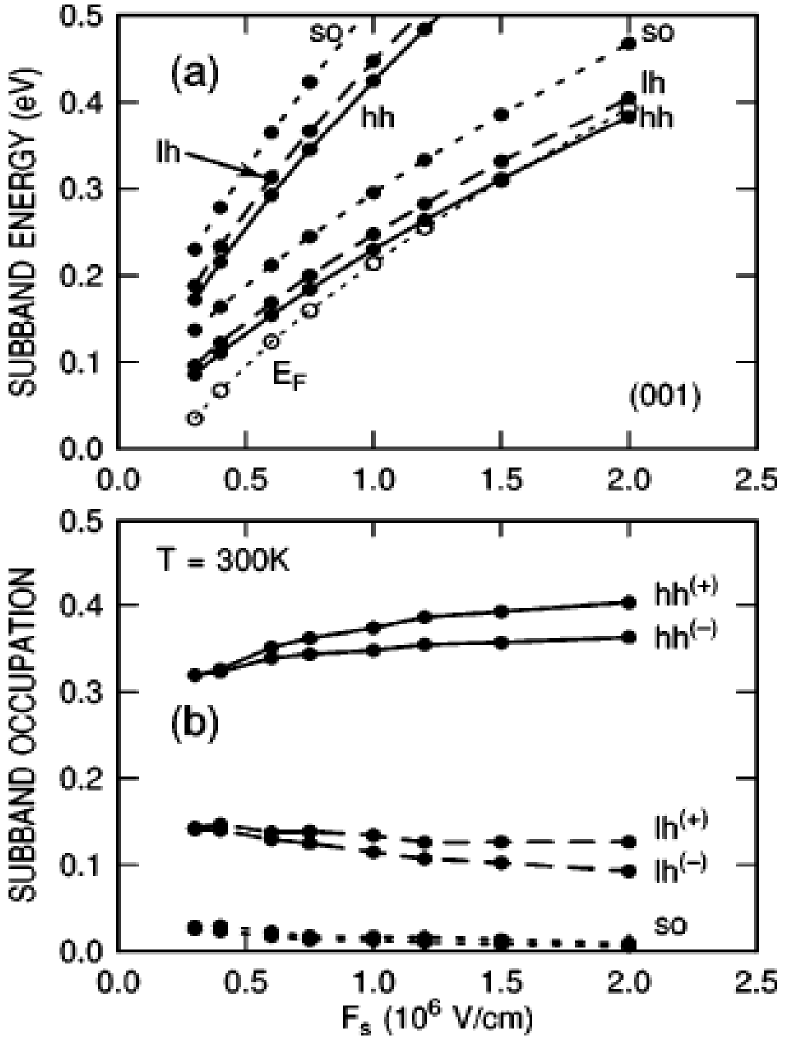
$$[H(\vec{K},k_z)+\mathrm{I}V(z)]\psi_{\vec{K}}(z)=E(\vec{K})\psi_K(z)$$

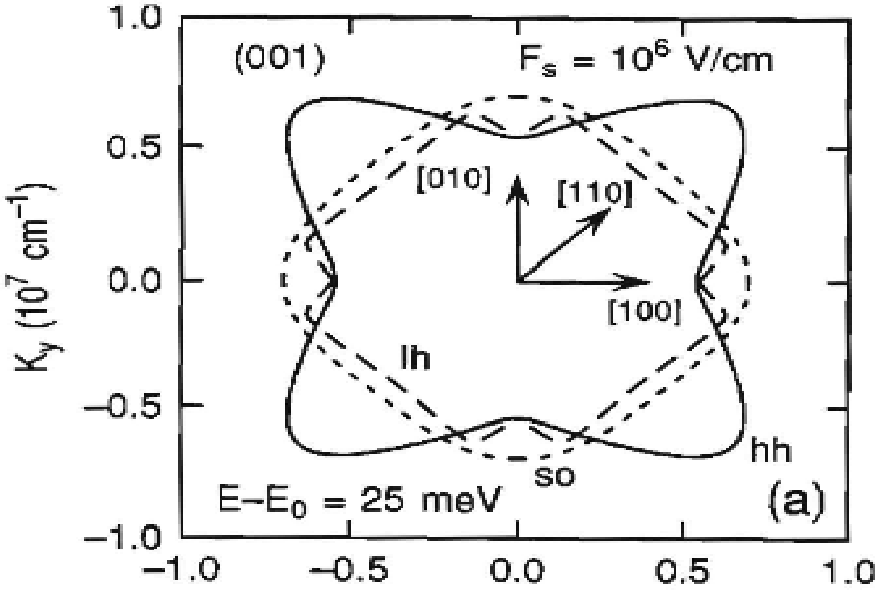
$$\partial_z^2 V_H(z)=-\frac{e^2}{\in_g}[\rho(z)-\rho_e z+N_D(z)]$$

- Use “triangular-well” approximation: $V(z)=eF_s z$
- Works well for Si (Fischetti et al., J. App. Phys., 2003)
- After calculating scattering probabilities, use Monte-Carlo to model hole motion.

Surface Valence Band Models

(Fischetti et al., J. App. Phys., 2003)





- Surface potential gives rise to band splitting
- Phonons can scatter holes into various sub-bands

A Simple Surface Valence Band Model (2D)

- Consider the 3D warped band model evaluated at: $\theta = \pi/2$

$$\epsilon(\mathbf{k}) = \frac{\hbar^2|A|}{2m}k^2[1 \mp g(\theta,\psi)]$$

- This assumes a surface normal of 100 (100 and 010) are equivalent
- Calculate scattering probabilities in 2D (use 2D DOS)
- E.g., acoustic phonons give:

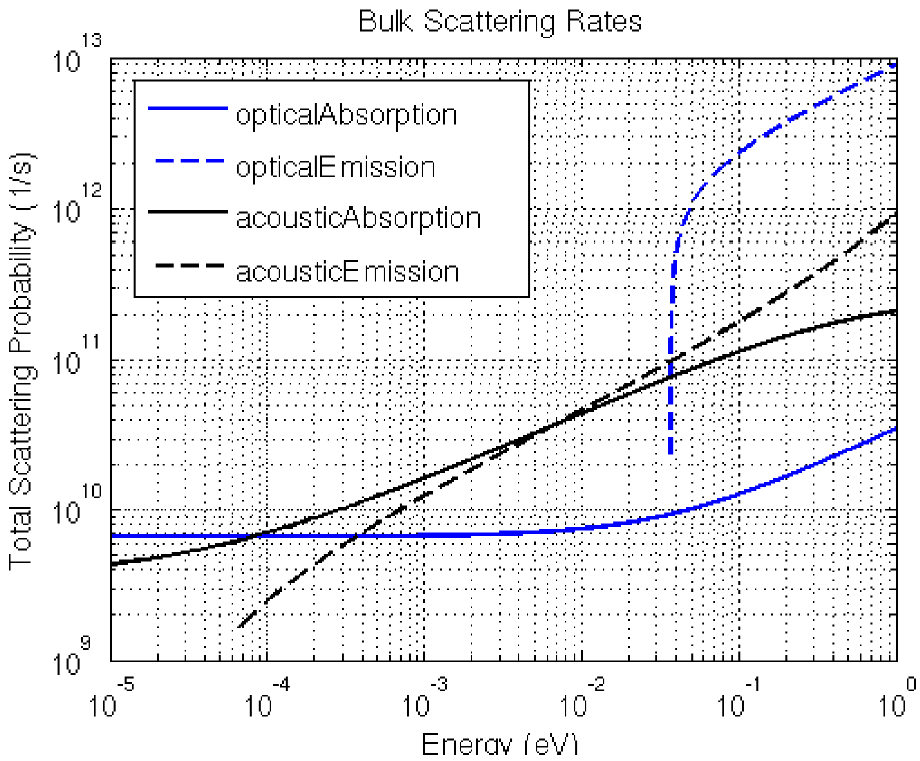
$$P(\vec{k},\vec{k}') = \frac{\pi q \zeta^2}{4V\rho u}\begin{pmatrix} N_q \\ N_q + 1 \end{pmatrix}(1 + 3\cos^2(\theta))\delta[\varepsilon(\vec{k}') - \varepsilon(\vec{k}) \mp \hbar q u]$$

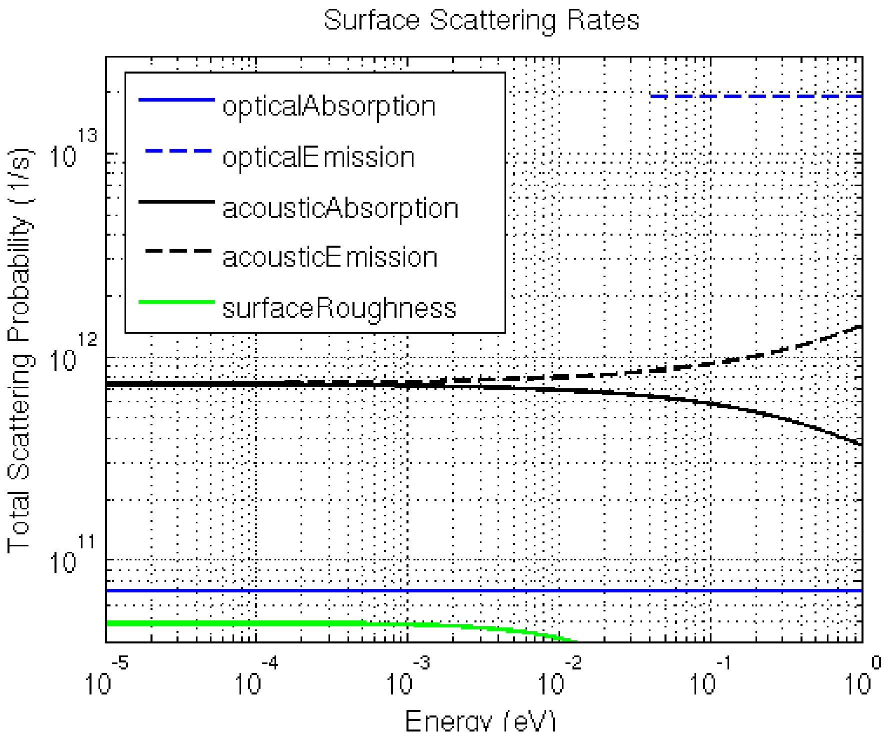
$$P(\vec{k},\psi') = \int P(\vec{k},\vec{k}')k'dk'$$

$$V = (2\pi)^2\Delta$$

Simple Surface Valence Band Model

- Repeat for optical phonons and surface roughness.

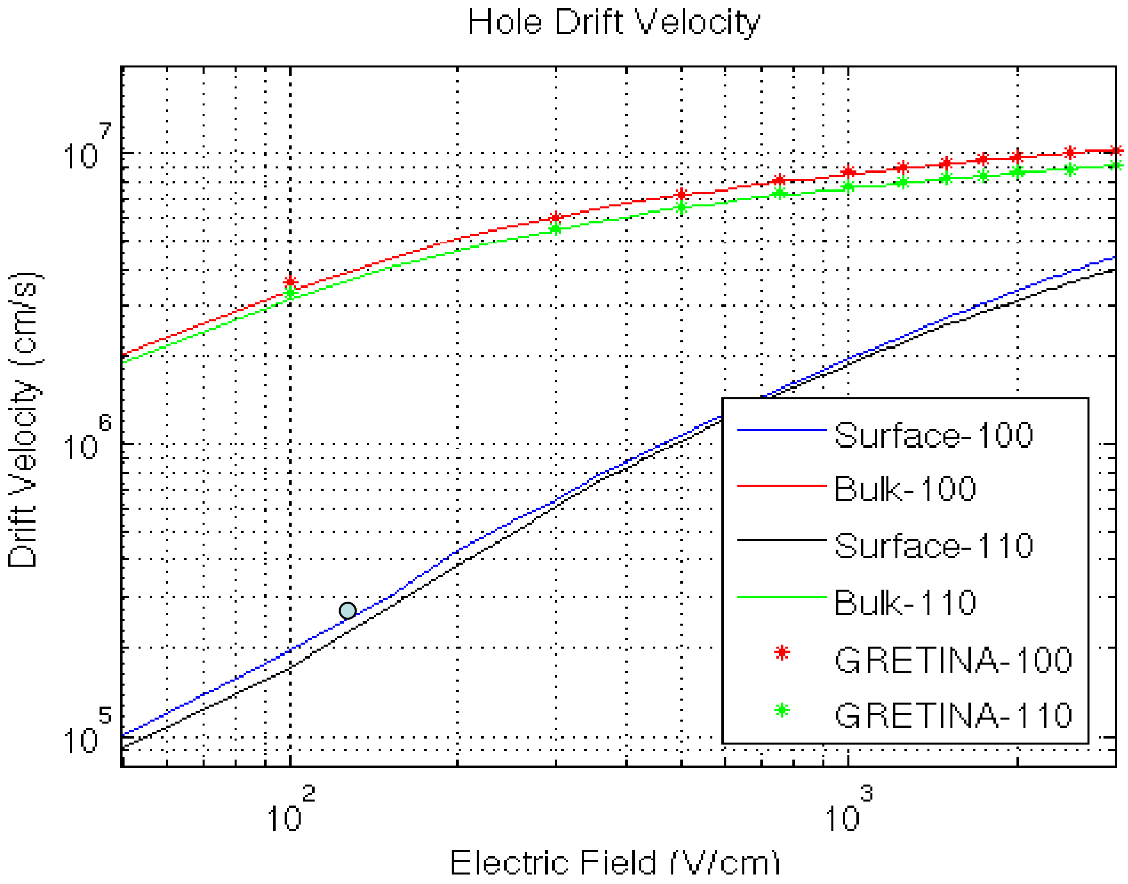




- Optical emission has an absolute cutoff
- Effect from surface roughness is small

Simple Surface Valence Band Model

- Drift velocity shows substantial changes.



- PPC detector surface radial E-field 125 V/cm; Vd=2.5*10^5 cm/s

Conclusions

- Reduction in surface mobility because of fundamental changes in phonon scattering
- Surface effects change with delta (for model considered here).
- Simple models can yield insight into the surface behavior

Current and future work

- Implementing interband scattering between heavy and light bands
- Integrating more accurate band non-parabolicity for simple warped band model (energy dependent effective mass)
- Developing surface subband calculations (triangular well appx) for Ge and coupling into Monte Carlo simulations (VORPAL)
- Need to validate results with more experimental data to from PPC and GRETINA detectors
- Overall result will be → better signal modeling for GRETINA=better resolution = better physics