Computational Models of Germanium Point Contact Detectors

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Modeling of Signal Generation in Gamma Ray Detectors
Office of Nuclear Physics

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GPU-Acceleration of EM (PIC) Simulations

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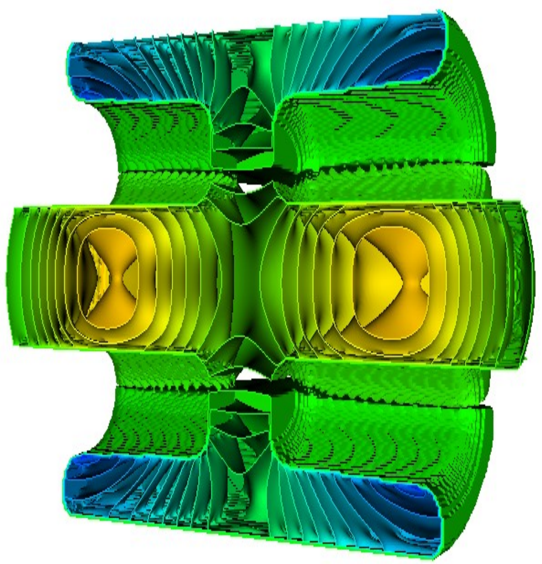
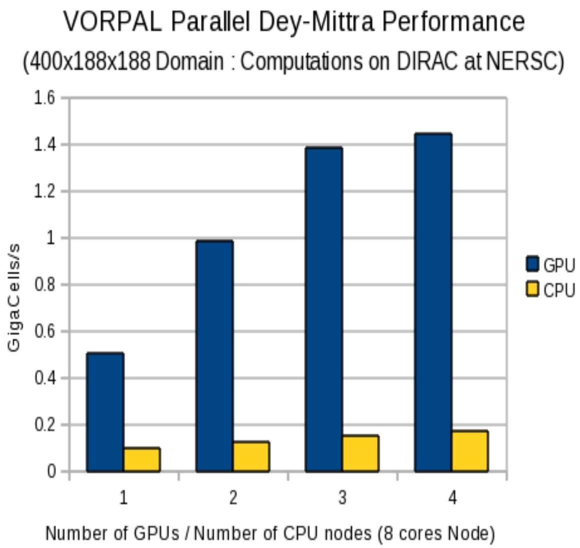
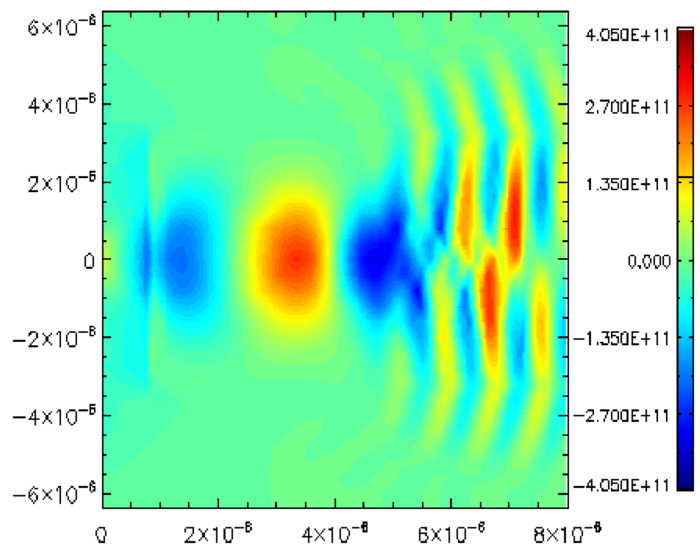
- Dey-Mittra solvers for complex geometries
- Arbitrarily complex space-time functions (at run-time) enable simulations of dielectric structures
- Prototype EM-PIC algorithm shows big acceleration over traditional CPU-based implementations



EM Crab Cavity Simulation



EM Dey-Mittra Performance



EM PIC LWFA Simulation

Phase II Project Description

Title:

"Modeling of Signal Generation in Gamma Ray Detectors"

Objectives:

- Develop models and tools for computing carrier mobility in detector crystal bulk and surfaces.
- Develop tools for accurately computing the electric fields around detector surface.

Abstract

In the crystal bulk of group IV covalent semiconductors such as germanium (Ge), simple analytic models for the valence band structure can provide fast, accurate computations of hole mobility for moderate energy ranges up to a few eV. On the surfaces of these materials, such as on Ge-vacuum or Ge-GeO2 interfaces, the transport rates differ significantly from the bulk. This can be problematic for both point contact and segmented Ge gamma ray detectors, that require accurate carrier drift rates for computing signal basis sets, which themselves are necessary for the precise determination of gamma-ray induced compton scattering events. While several techniques exist for computing surface hole mobilities, more often than not, these methods are complex to implement, require significant computational resources, and lack the simplicity of bulk models for interpreting results. This talk presents a new technique for computing Ge surface hole mobility that can give a first estimate for the surface transport rates after tuning a physically-based computational parameter. This model is used in conjunction with particle-in-cell (PIC) simulations for modeling hole-dynamics inside a Ge p-type point contact detector. The results of our calculations agree with experimental data gathered from Ge p-type point contact detectors at Oak Ridge National Laboratory.

(1) P. Mullowney et al, Nucl. Instr. and Meth. A (2011) doi:10.1016/j.nima.2011.09.061

(2) R.J. Cooper et al, Nucl. Inst. and Meth. A (2011), submitted

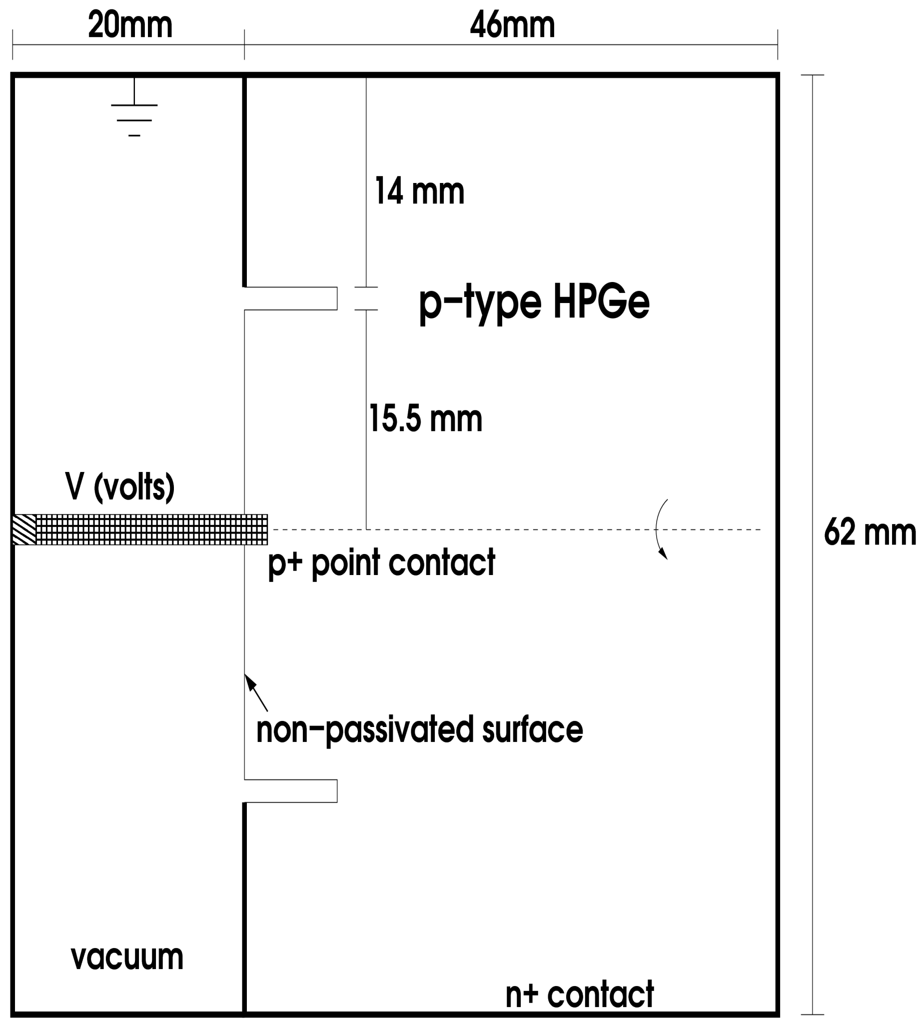
HPGe Point Contact Detector

Work done by D.C. Radford and R.J. Cooper at ORNL.

- Candidate gamma-ray detector for Majorana collaboration's double beta decay experiment.

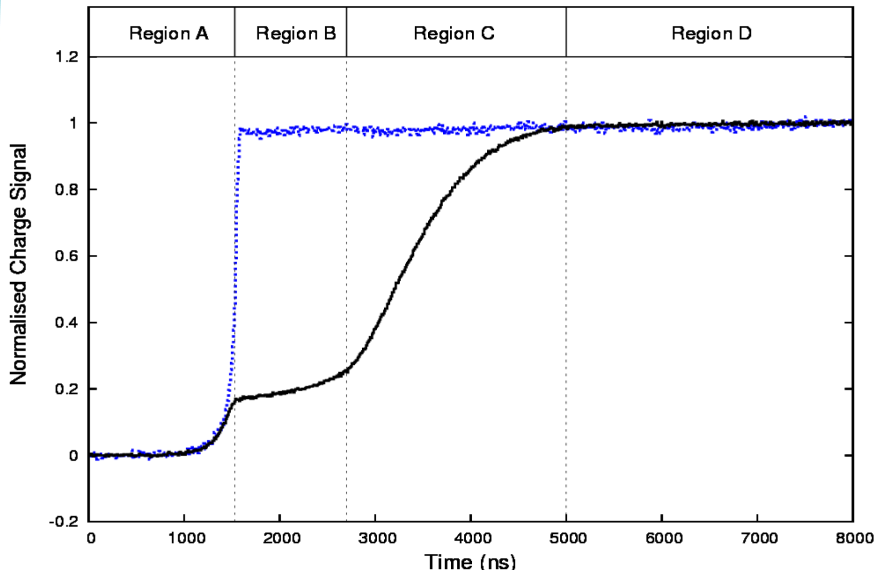
- Cylindrically symmetric, high-purity Germanium (HPGe), P-type detector enables
  - precise energy resolution
  - good background rejection performance
  - refined multi-site interaction detection

- The depletion voltage of the device is observed to change on the time scale weeks!



PC Detector Signals

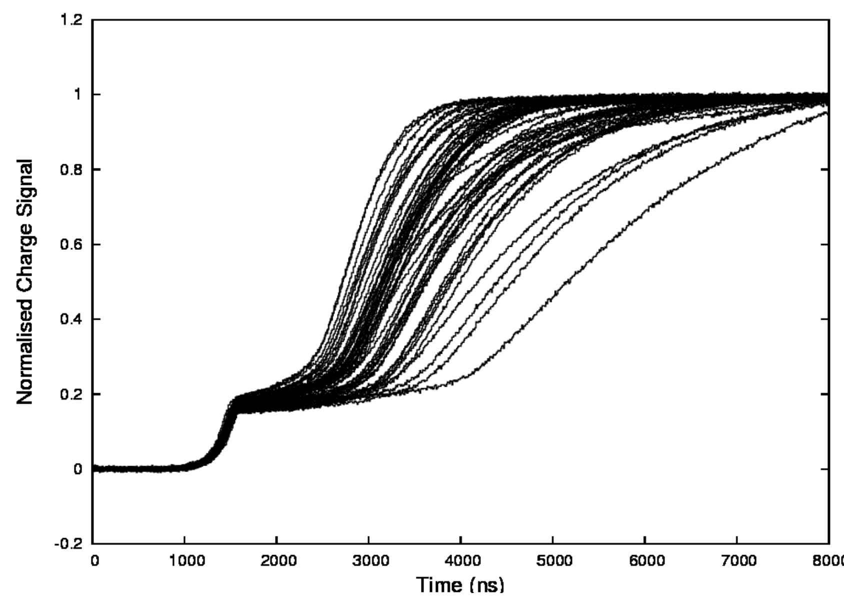
Work done by D.C. Radford and R.J. Cooper at ORNL.



Region A : Normal bulk charge motion
Region B : Charge hits surface
Region C : Acceleration on surface showing impaired motion
Region D : Pulse reaches a maximum

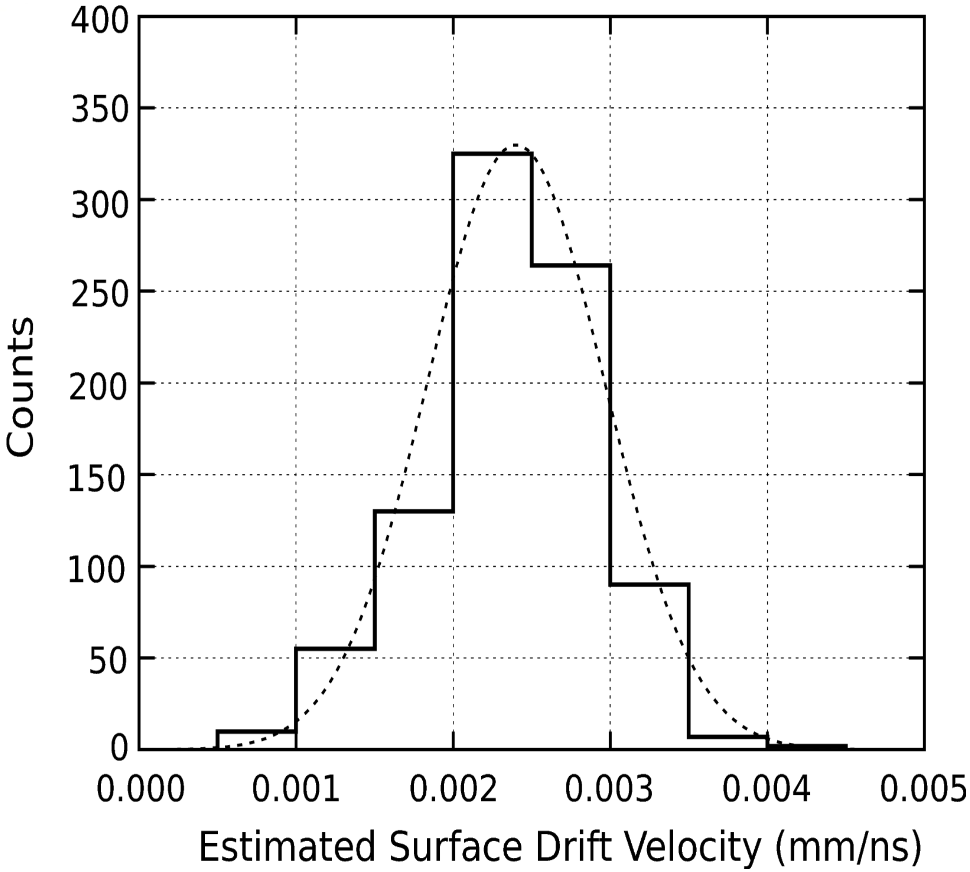
Above : a typical example of an anomalous signal recorded when the detector was operated just over depletion. For comparison, a signal representing the typical, bulk response of the PC detector is overlaid (dashed blue line).

Right : A collection of pathological signals. Spread of signals once they hit the surface is thought to be due to diffusion.



Drift Velocity Estimation

Work done by D.C. Radford and R.J. Cooper at ORNL.



- Histogram of the value of radial drift velocity estimated from one thousand anomalous events.
- Performing a Gaussian fit to the data (shown by the dashed black line) yields a mean value of

$$v_{drift} \sim 2.4 * 10^{5}\, cm/s$$

- Estimated surface drift is a factor of 40 slower than the accepted value for hole saturated drift rate in bulk HPGe

Detector Model

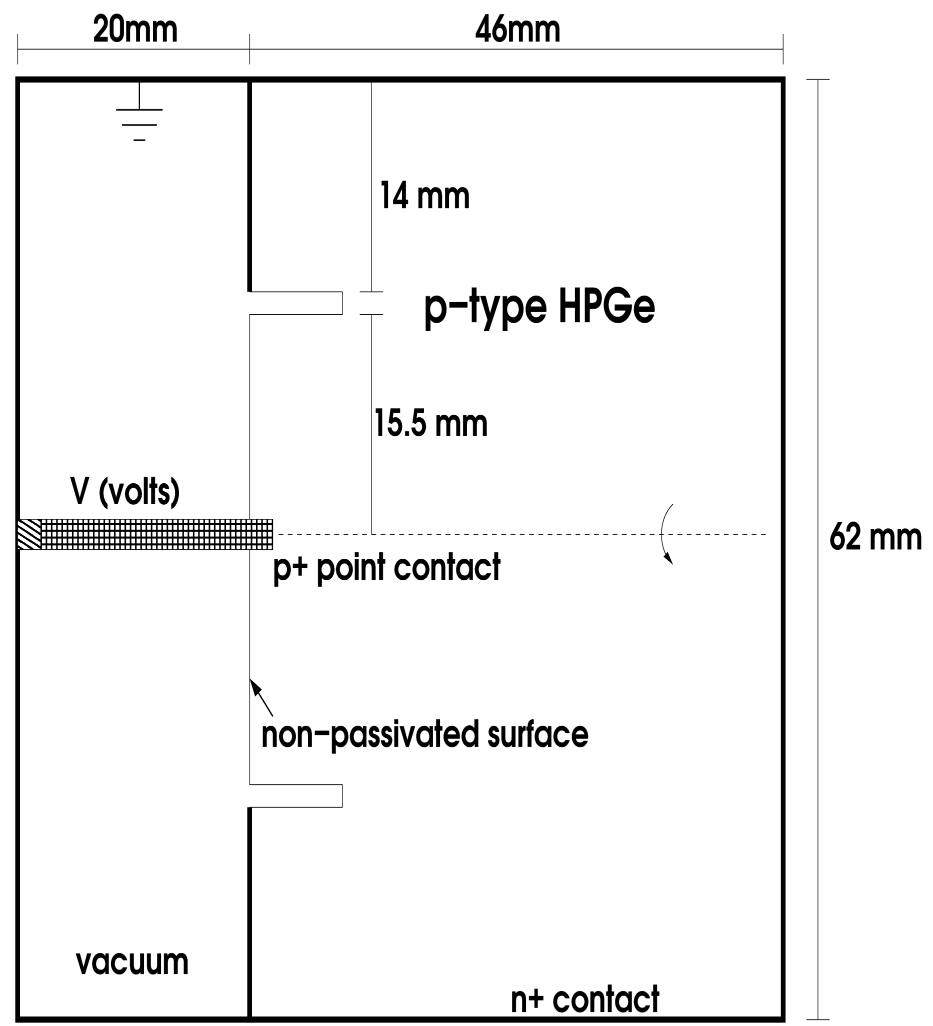
- Long time scale change in depletion voltage is thought to be due to accumulation of surface charge:

  We place a layer of stationary, uniformly distributed placed on the non-passivated surface (free parameter of simulation).

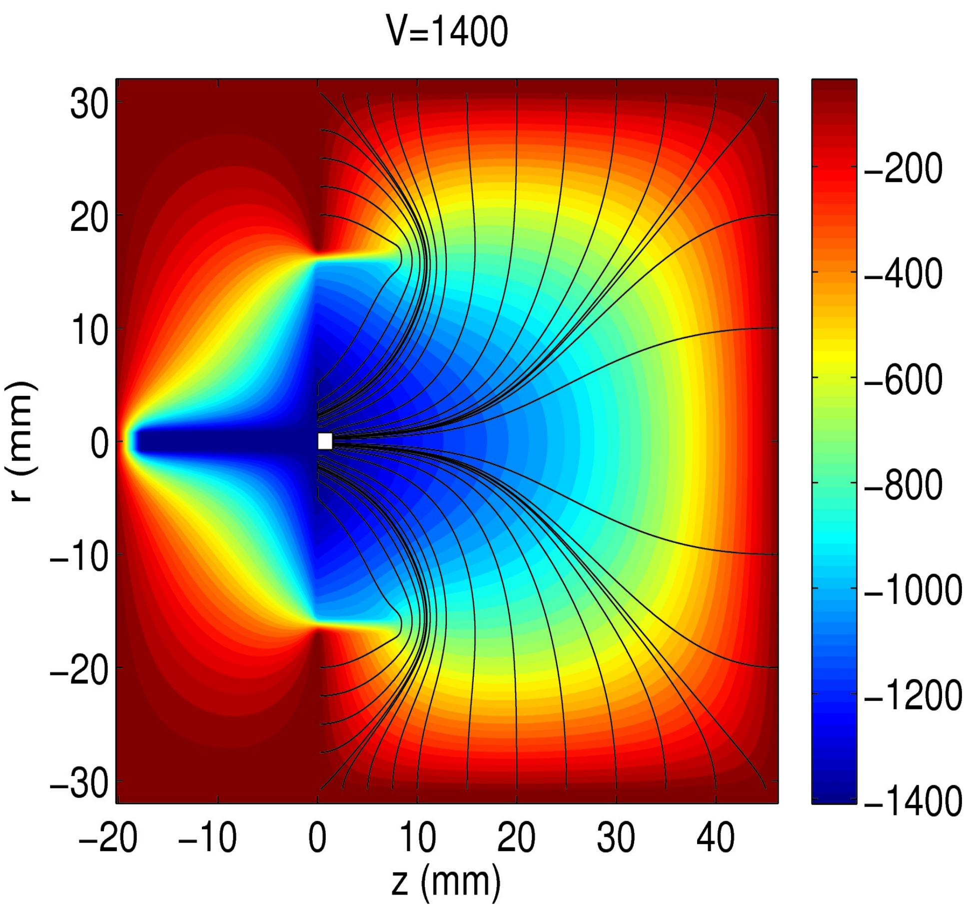
- Stationary distribution of (negatively charged) impurities placed in crystal bulk.

- Point contact is modeled as a wire extending into the vacuum:

  Voltage of the wire is quickly brought to 0 linearly at the left most ground plane (operational parameter of the detector).



Detector Model



$$N_x = N_y = 256, N_z = 266, N_t = 10^4$$

- Quasi self-consistent simulations done in VORPAL PIC code.
- Electric field computed every 100^{th} time step in parallel. Cylindrical boundary is handled through stair-stepping.
- Hole trajectories (black lines) are computed via look-up tables, i.e. parameterized tables of v_{100}, v_{110}, v_{111} versus electric field in bulk and on surface.

  What is the surface drift velocity?
- Look-up table captures hole trajectory anisotropy.

Simple Surface Valence Band Models

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

$$\epsilon(\mathbf{k}) = ak^2 \left(1 - \sqrt{b^2 + c^2 \cos^2 \psi \sin^2 \psi}\right)$$

- Colman et al (1968) employed a similar trick, but they evaluated at

$$k_z = \pm \frac{\sqrt{2m|\epsilon_0|}}{\hbar}$$

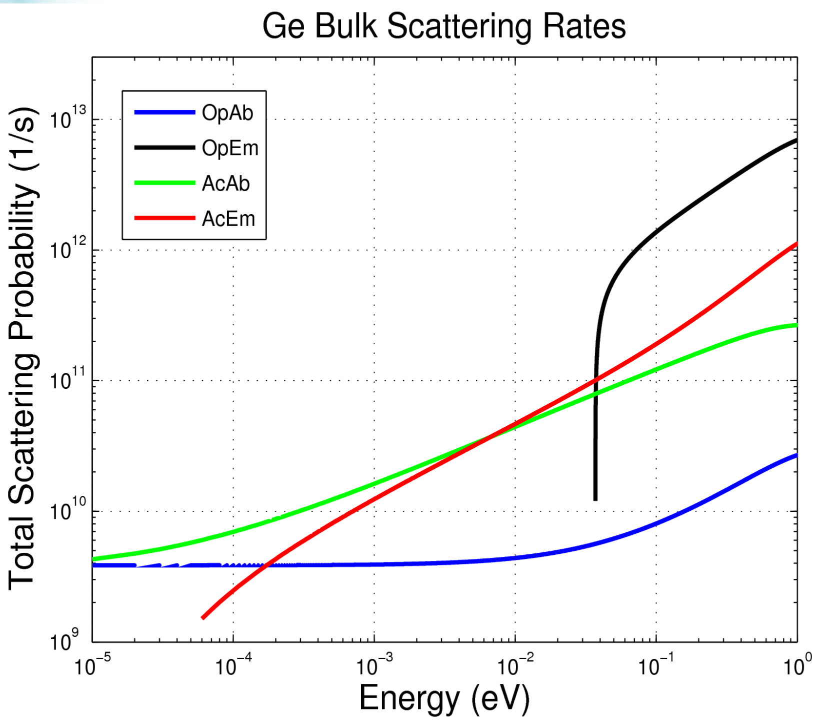
- 2D scattering probabilities are given by integrating

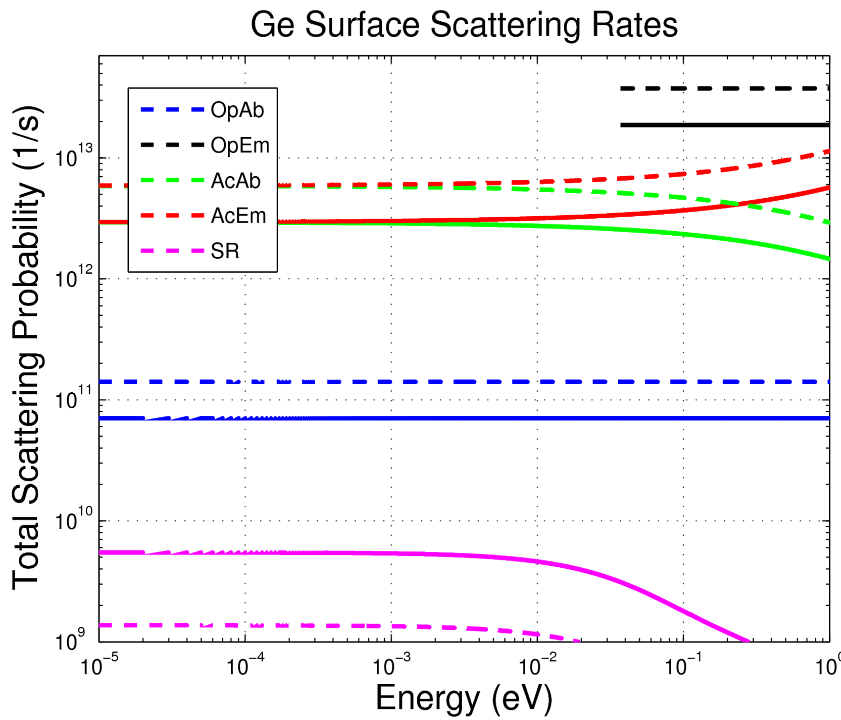
$$P\left(\mathbf{k}, \psi'\right) = \frac{V_{2DEG}}{(2\pi)^2 \Delta} \int_0^\infty P\left(\mathbf{k}, \mathbf{k}'\right) k' dk'$$

$$P_{ab,em}\left(\mathbf{k}, \mathbf{k}'\right) = \frac{\pi q \mathcal{E}^2}{4V\rho u} \begin{pmatrix} N_q \\ N_q + 1 \end{pmatrix} \left(1 + 3\cos^2\theta\right) \times$$

$$\delta\left[\epsilon\left(\mathbf{k}'\right) - \epsilon\left(\mathbf{k}\right) \mp \hbar q u\right] \ .$$

Simple Surface Valence Band Models

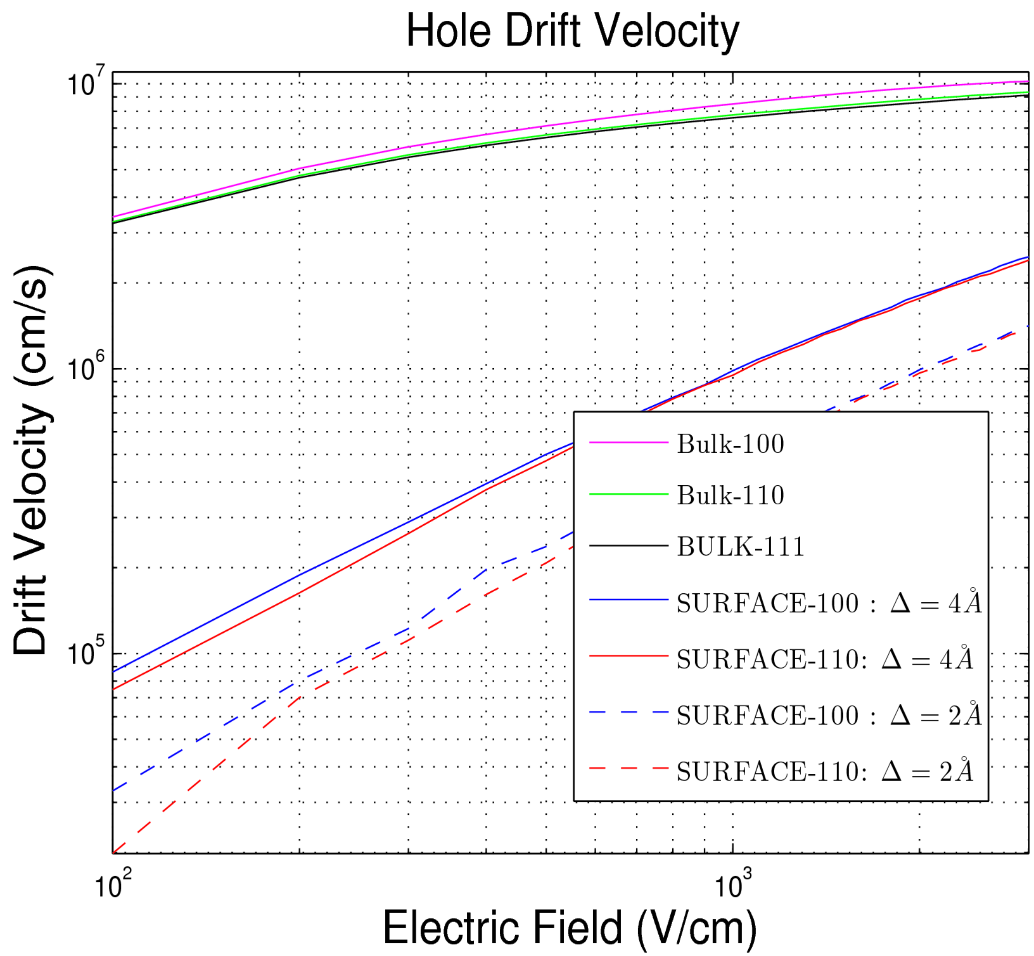




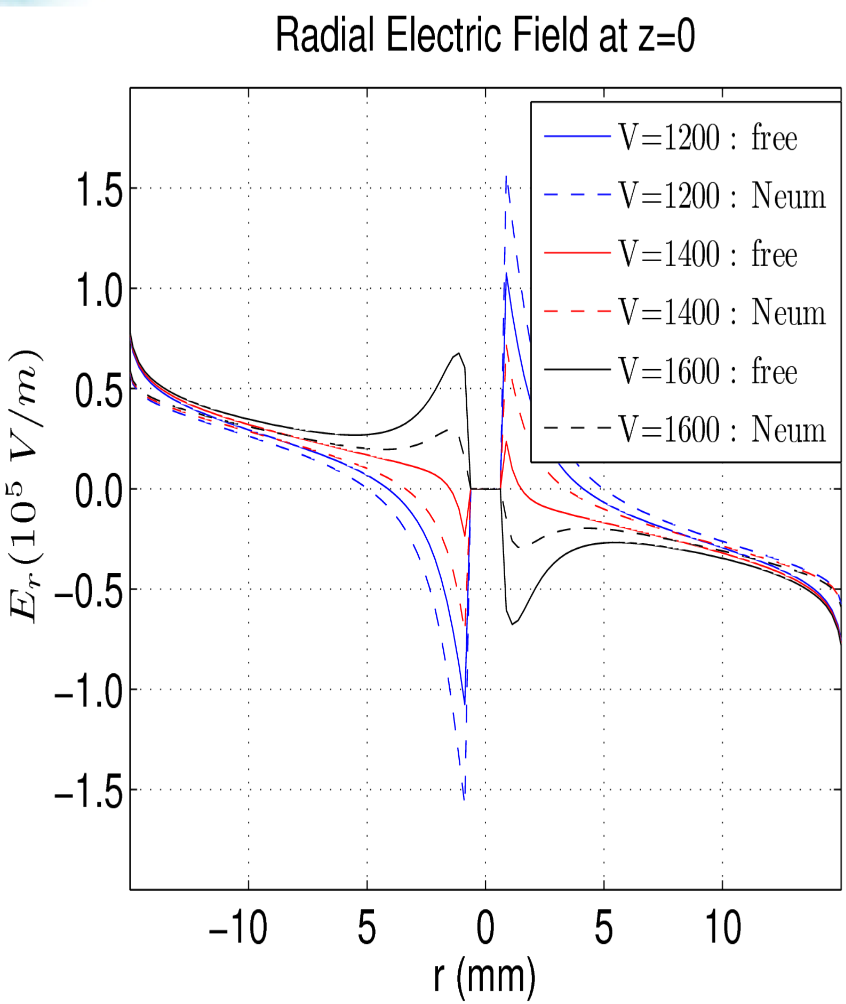
- Scattering rates are substantially higher.
- Optical emission has an absolute cutoff (in bulk and on surface).
- Surface roughness is negligible, even at high fields $E_r \sim 3*10^6 Volts/m$.
- Typical values of Δ are estimated to be between 2$\mathring{A}$ (dashed lines) to 4$\mathring{A}$ (solid lines).

Simple Surface Valence Band Models

- Use standard Monte Carlo technique (Jacoboni et al. 1983) coupled to self consistent ES Solve.
- Drift velocity shows substantial changes.
- Δ is a free parameter. It represents the thickness of the surface layer.
- Bulk computations are consistent with the literature.



Surface Drift Velocity Estimation



- We computed the surface radial electric field versus the applied voltage at the point contact

  "Negative" electric fields denote undepleted regions in the crystal. Full depletion occurs when the detector capacitance is minimized.

  Above the depletion voltage, electric fields are on the order of

  $$E_r \sim 3*10^4\,Volts/m$$

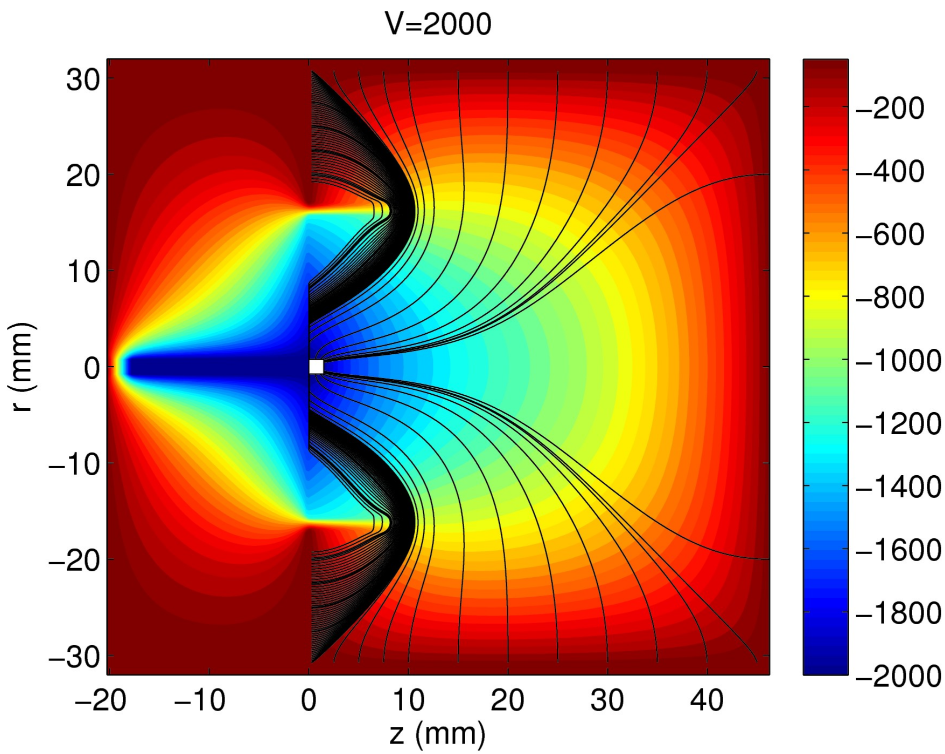
  Parameterized drift velocity calculations leads to an estimate of

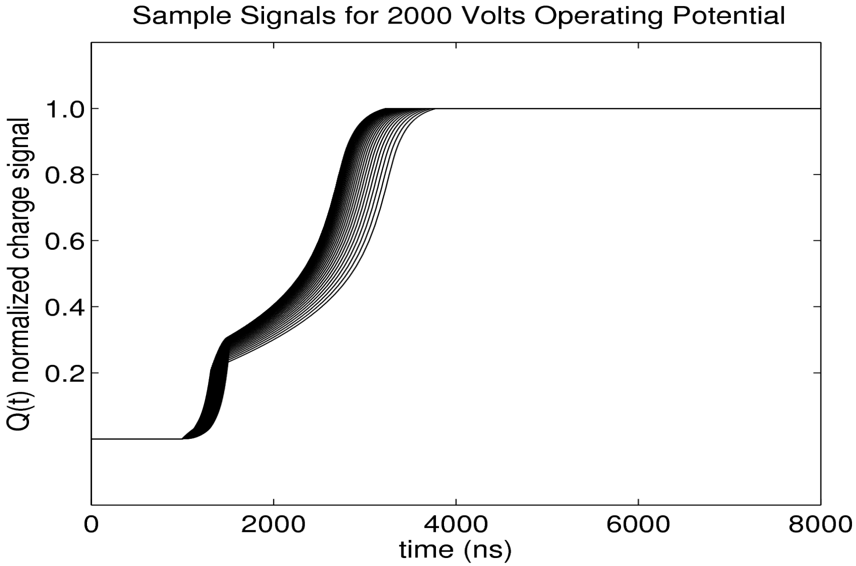
  $$v_{drift} \sim 2*10^5\,cm/s$$

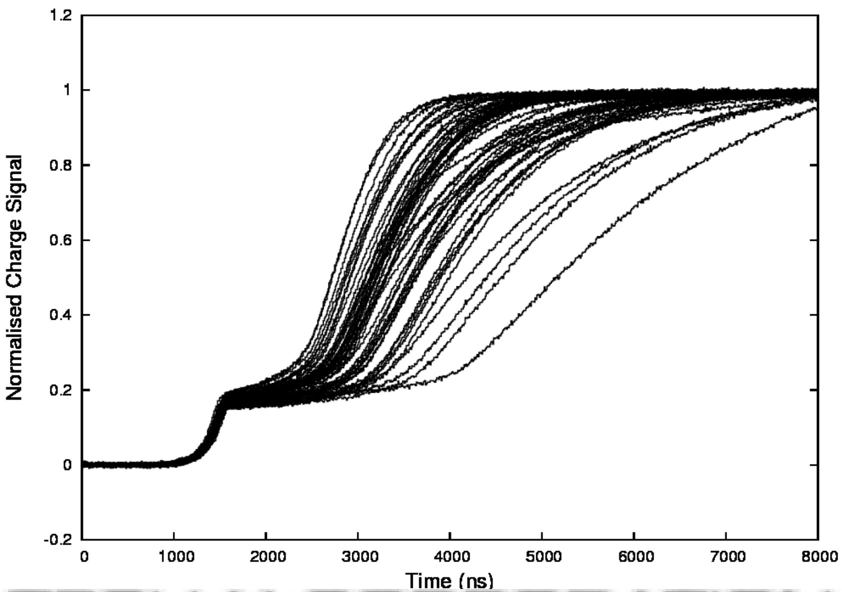
Signal Simulation

Simulated signals show the same qualitative features as the measured signals!

Need to study the parameter space (surface charge density) and add diffusion effects to get quantitative agreement.







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Conclusions

- Reduced models for can provide key insight into the behavior of holes on detector surfaces.
- Whole device simulations can be efficiently performed which capture key characteristics of device behavior.
- Even if you don't believe the reduced model, VORPAL can still be used to do whole device simulations. You have to supply your own tabulated drift velocities.

Phase II Project Summary

- Successful Phase II project resulting in novel computational models, experimental corroboration, new VORPAL simulation tools, and good collaboration between industry and lab!
- Beneficial work for DOE Office of Nuclear Physics!

Future Work

- Valid with more experimental data from GRETINA detector
- Employ strategy to other detectors or Group IV semiconductor devices made from Silicon, Diamond, ...

Warped Band Model

- 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, i.e. material speed of sound, temperature, density, ...

- Cyclotron resonance experiments are used to calculate the band parameters.

- Density of states calculations reveal that heavy hole has ~95% occupation, the light hole has ~5% occupation, and the spin orbit has ~.01% occupation.

Surface Valence Band Models

- One can work **very** hard to calculate the valence band structure accurately in surface inversion layers (Fischetti et al., J. App. Phys., 2003)

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

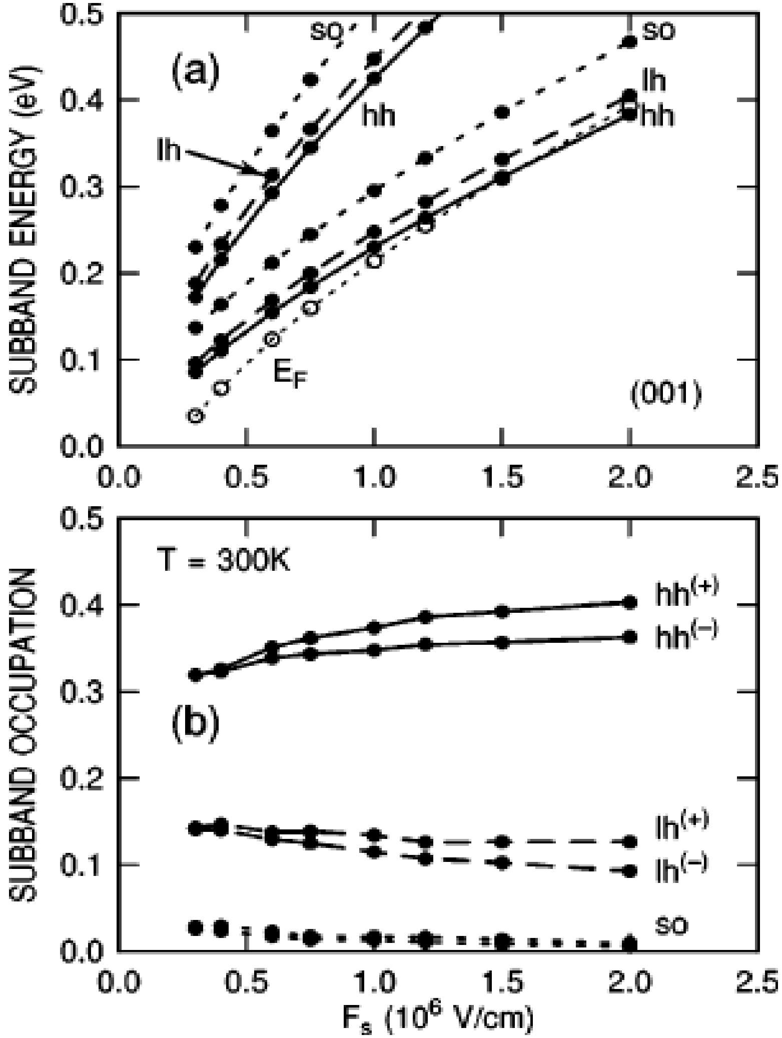
$$\partial_z^2 V_H(z)=-\frac{e^2}{\epsilon_g}[\rho(z)-\rho_e z+N_D(z)]$$

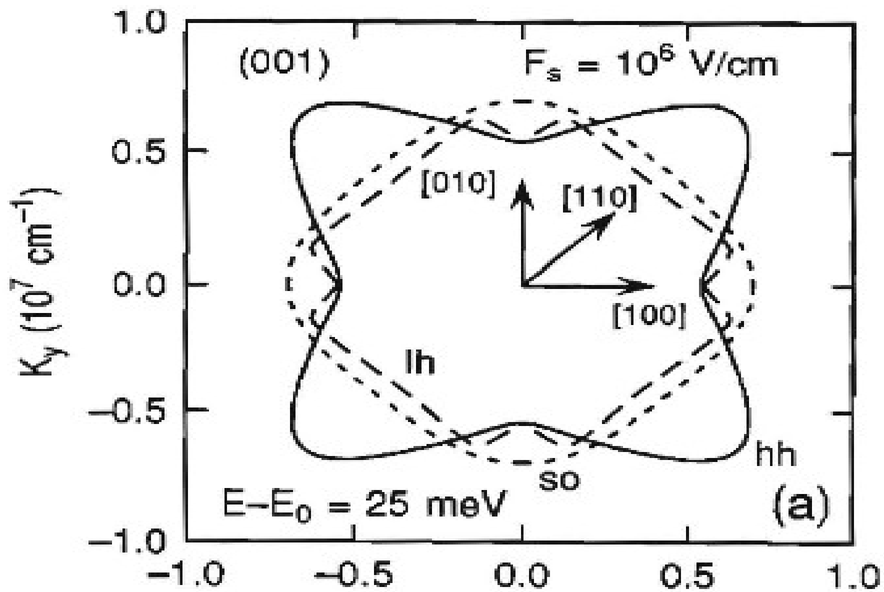
- Couple an Eigenvalue and ES solve (in surface normal direction) in order to get the dispersion relation (under the “triangular-well” approximation :

$$V(z)=eF_s z$$

- Boundaries conditions require care.
- After calculating scattering probabilities (relaxation times), one can use Monte-Carlo and PIC to model hole motion.

Surface Valence Band Models





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