Multiscale 3D Simulations of Charge Gain, Transport, and Collection Efficiency in Diamond

(initial simulations with electron emission)

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Work funded by the U.S. DOE office of Nuclear Physics under SBIR
Grant # DE-FG02-06ER84509

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Work in BNL funded under U.S. DOE
grant # DE-AC02-98CH10886

Acknowledgements: Kevin Jensen, NRL

Outline

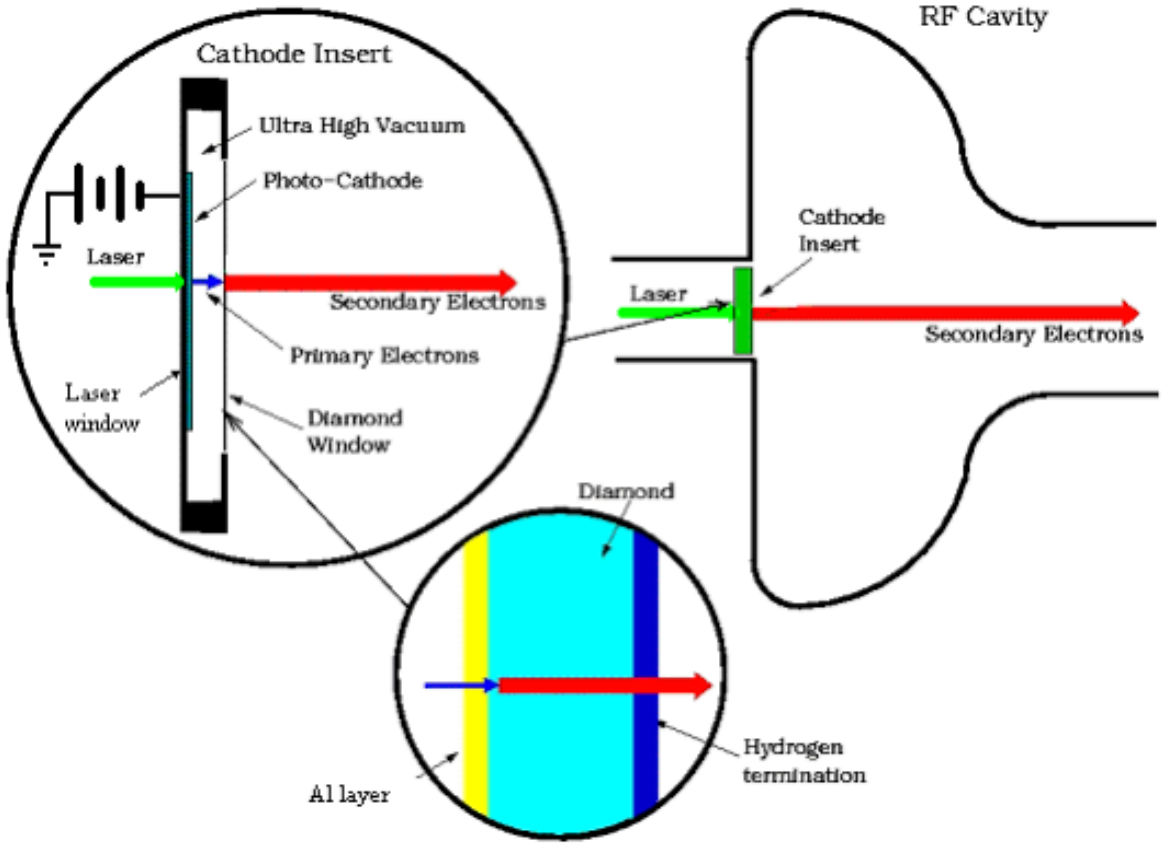
- Motivation
  - Diamond-amplifier cathode concept & types of experiments
  - Diamond-based beam line detectors
- Models developed in VORPAL to simulate diamond amplifier & detector physics:
  - Secondary electron generation
  - Electron-phonon and hole-phonon scattering for simulation of charge transport, charge impurity scattering
- Results
  - Verification of the developed models for the underlying physics
  - Comparison of simulation results to data from transmission-mode experiments
  - First simulations of a diamond-vacuum system and electron emission
  - Initial modeling of collection efficiency for x-ray detectors
- Summary

Motivation

- A new diamond-amplified cathode was proposed recently with the potential to provide *high quantum efficiency* sources with *very long lifetime* for generation of *high-current*, *high-brightness*, and *low emittance* electron beams.
- Experiments have demonstrated the potential of the concept but the optimal design and parameters of operation are still being investigated.
- We are developing models, within the VORPAL 3D particle-in-cell code, to simulate physical properties of diamond-amplified cathodes and detectors.
- Our goal is to explore relevant parameters via computer simulations to provide additional understanding how to produce diamond-amplified cathodes and detectors with optimal physical properties.

Overall Diamond-Amplifier Concept

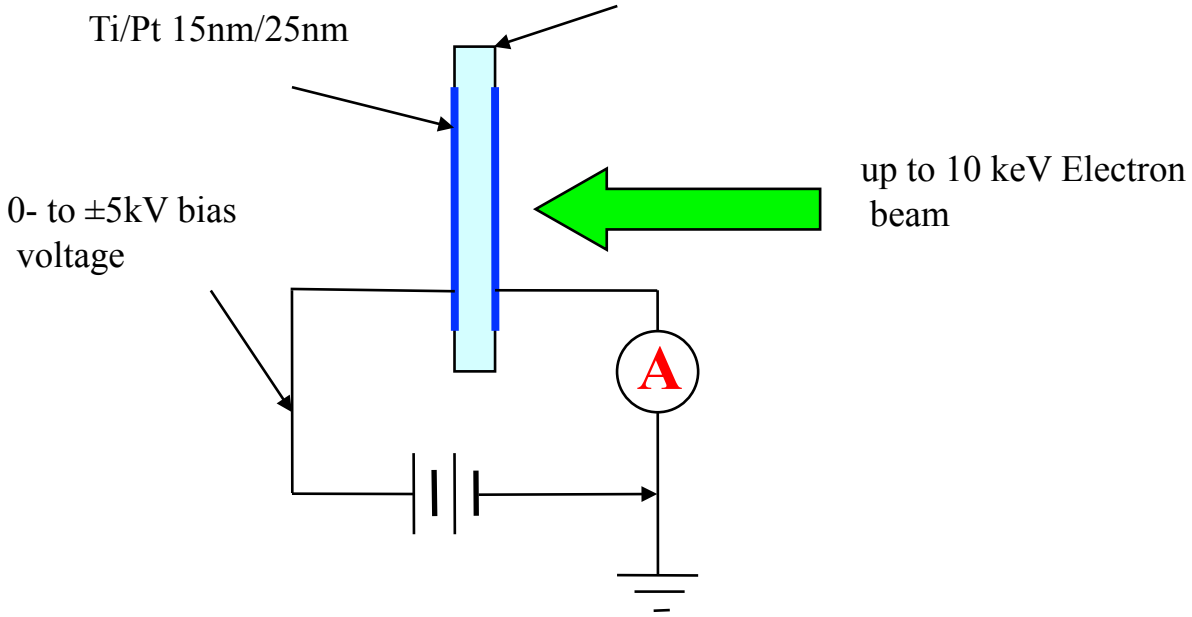
- The overall concept includes:
  - a drive laser for primary electrons
  - a diamond sample for electron charge amplification
  - RF cavity for acceleration of electrons from the diamond emitters



Schematic diagram of a secondary emission enhanced photoinjector (SEEP)

Diagram courtesy of Triveni Rao, BNL.

Electron generation and gain is measured in transmission and emission mode experiments.



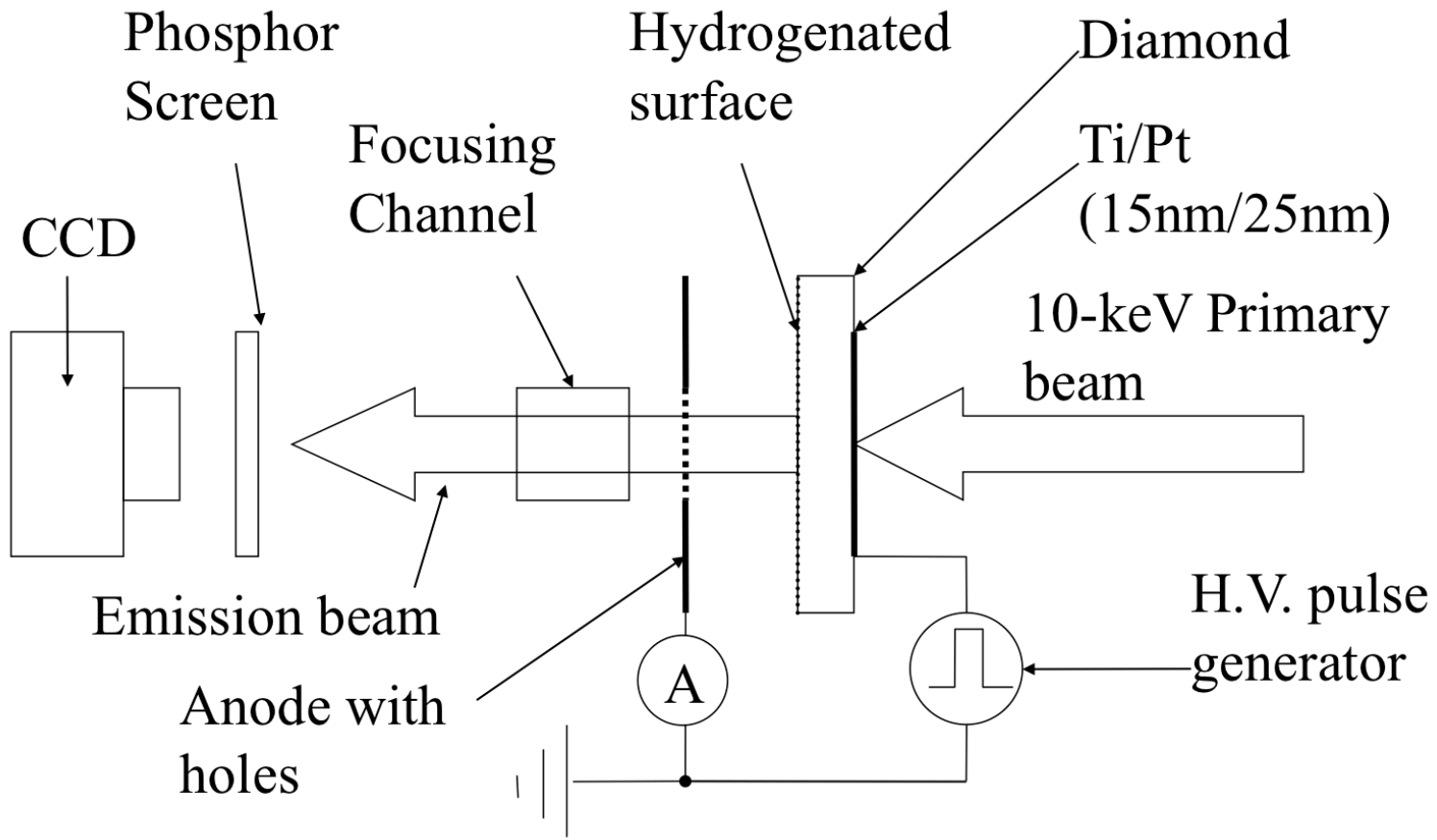
DC Transmission-mode Experiment

diagram courtesy of Xiangyun Chang, BNL

- Electron current transmitted in response to primary electrons is measured.
- Metal contacts are applied to opposite surfaces of diamond to apply an external field and collect generated charge carriers.

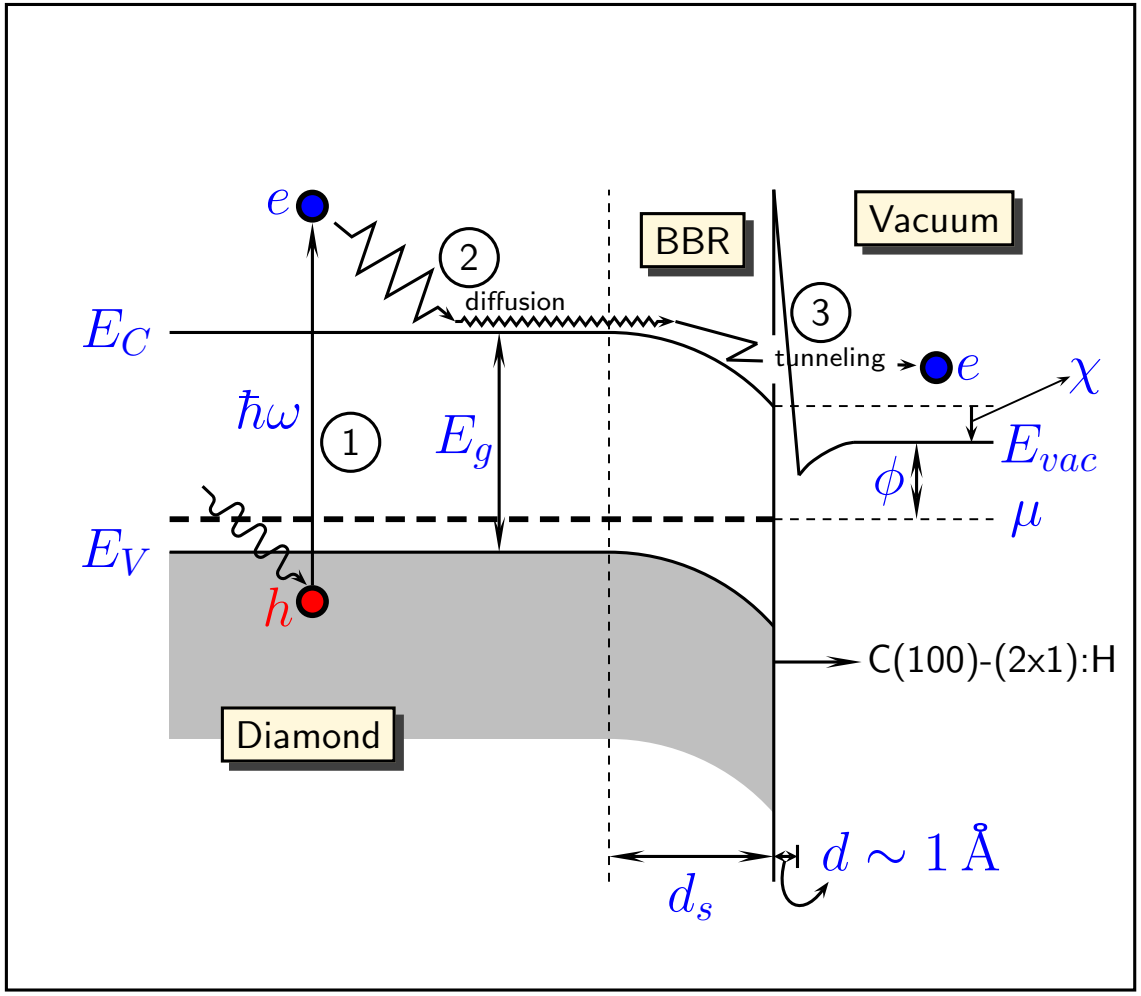
Electron emission from diamond was measured recently.

- Maximum electron gain of 40 was demonstrated recently in emission-mode experiments (Xiangyun Chang *et al.*, to be published in Phys. Rev. Lett.):



There are three main phases to model.

1. Secondary electron generation
2. Charge transport
3. Electron emission from diamond surfaces with varying electron affinity



New capabilities in the VORPAL code for modeling diamond properties.

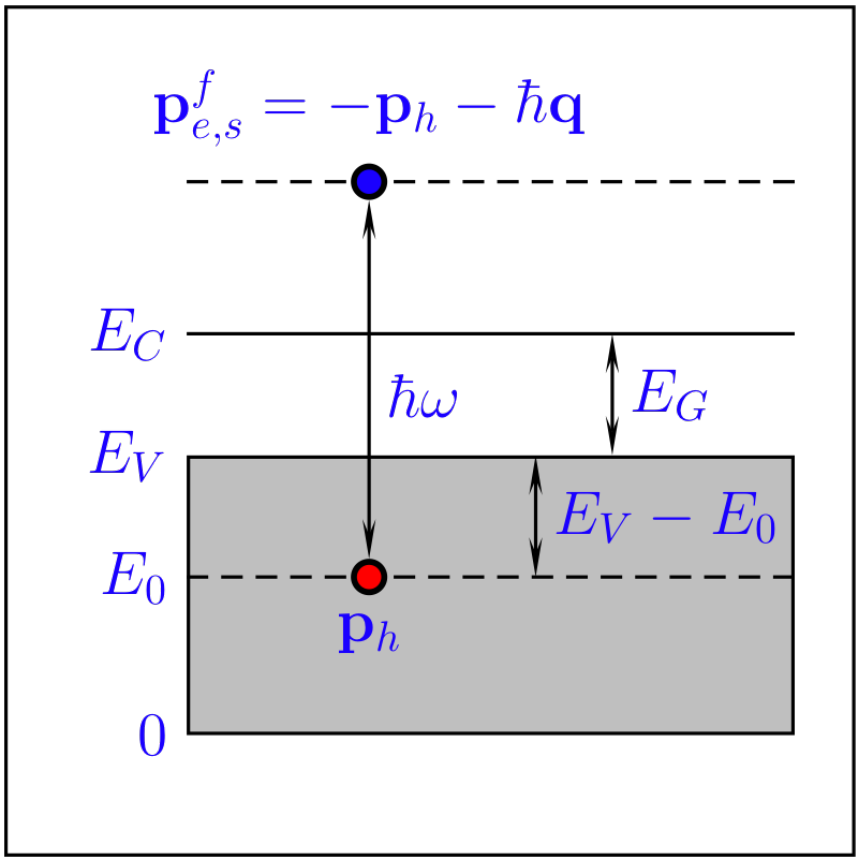
- To enable end-to-end simulations of diamond-amplified electron emitters we developed algorithms to model:
  - Inelastic scattering of electrons (primary & secondary) and holes for generation of electron-hole (e-h) pairs
  - Elastic scattering
    - at higher energies (> ~10 eV)
    - due to ionized impurities
  - Inelastic scattering with phonons
  - Code infrastructure for electron emission from diamond and a model for testing.
- VORPAL provides full electro-magnetic push of charged particles between scattering events.
- We implemented a general Monte-Carlo algorithm to handle charge particle scattering processes.

Secondary electron-hole generation

- The differential scattering cross section for electron-hole pair generation are calculated in VORPAL using the approach from:

  Ziaja et al., Phys. Rev. B 2001 & 2002, and J. Appl. Phys. 2005.

- *Both*, electrons and holes with $E_{kin} > E_G$ (5.47 eV) can generate electron-hole pairs.
- We implemented the Ashley and Tanuma-Powell-Pen (TPP) optical models for impact ionization scattering.



Calculation of the inelastic mean free path for impact ionization

- We implemented the TPP and Ashley optical models for calculation of impact ionization scattering.
- The probability for impact ionization is give by the total scattering rate (via the inelastic mean free path (IMFP)).
- The IMFP is calculated using the energy loss function (ELF) as the only input from:

$$\frac{1}{\lambda(E)} = \int_0^{E/\hbar} \tau(\omega, E)\, d\omega,$$

$$\tau(\omega, E) = \frac{\hbar}{\pi a_0 E} \int_{q-}^{q+} \frac{dq}{q} \int_0^{\omega} d\omega_p \frac{\omega_p}{\omega} \delta(\omega - \omega_p(q)) \operatorname{Im}\left(\frac{-1}{\epsilon(0, \omega_p)}\right)$$

Sampling for the energy change in impact ionization

- Given an electron with energy E is chosen for an inelastic scattering event, select ω (the energy lost by the electron) according to the probability density (pdf) function

$$p(\omega \mid E) = \frac{\int_{q-}^{q+} \frac{\partial^2 \sigma_{in}(q', \omega, E)}{\partial q' \partial \omega} dq'}{\int_{\omega_{min}}^{\omega_{max}} \int_{q-}^{q+} \frac{\partial^2 \sigma_{in}(q', \omega', E)}{\partial q' \partial \omega'} dq' d\omega'} \qquad q_{\pm} = k\left(1 \pm \sqrt{1 - (\omega/E)}\right)$$

obtained from the doubly differential inelastic cross section:

$$\frac{\partial^2 \sigma_{in}(q, \omega, E)}{\partial q \partial \omega} = \frac{1}{n\pi a_0 E q} \mathrm{Im}\left(-\epsilon^{-1}(q, \omega)\right)$$

- q is the magnitude of the scattered electron's momentum change, ε is the dielectric function for diamond, and the imaginary part is the energy loss function (ELF).

Momentum change sampling for impact ionization

- After a value for the energy loss is obtained, the code samples a value for the magnitude of the momentum change q of the primary electron, according to the probability distribution:

$$p\left(q \mid \omega,\, E\right) = \frac{\dfrac{\partial^2 \sigma_{in}(q,\omega,E)}{\partial q \partial \omega}}{\displaystyle\int_{q-}^{q+} \frac{\partial^2 \sigma_{in}(q',\omega,E)}{\partial q' \partial \omega} dq'}$$

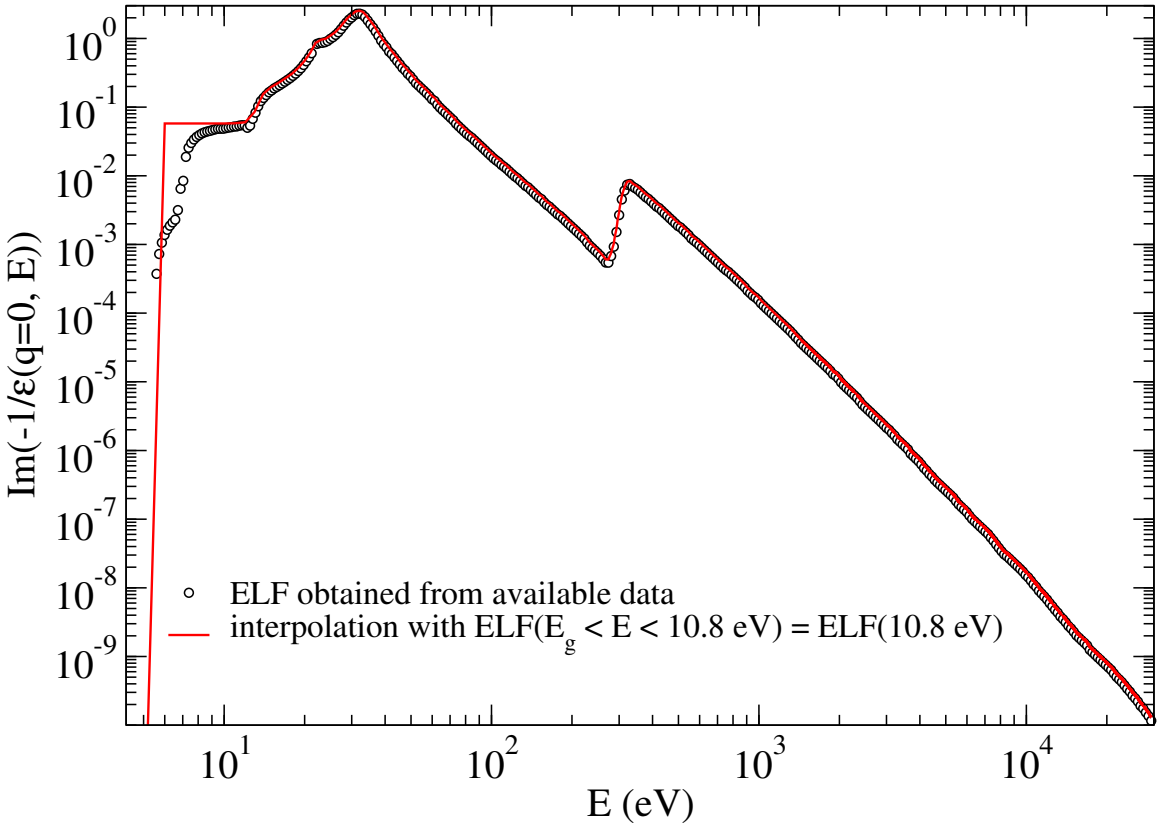
To support conservation of momentum for independently chosen E and ω values, q must satisfy:

$$\left|\left|\mathbf{p}_{e,s}^{i}\right| - \left|\mathbf{p}_{e,s}^{f}\right|\right| < q < \left|\mathbf{p}_{e,s}^{i}\right| + \left|\mathbf{p}_{e,s}^{f}\right|$$

- From E, the sampled ω and q, conservation of energy and momentum, the final momenta of the participating particles can be determined.

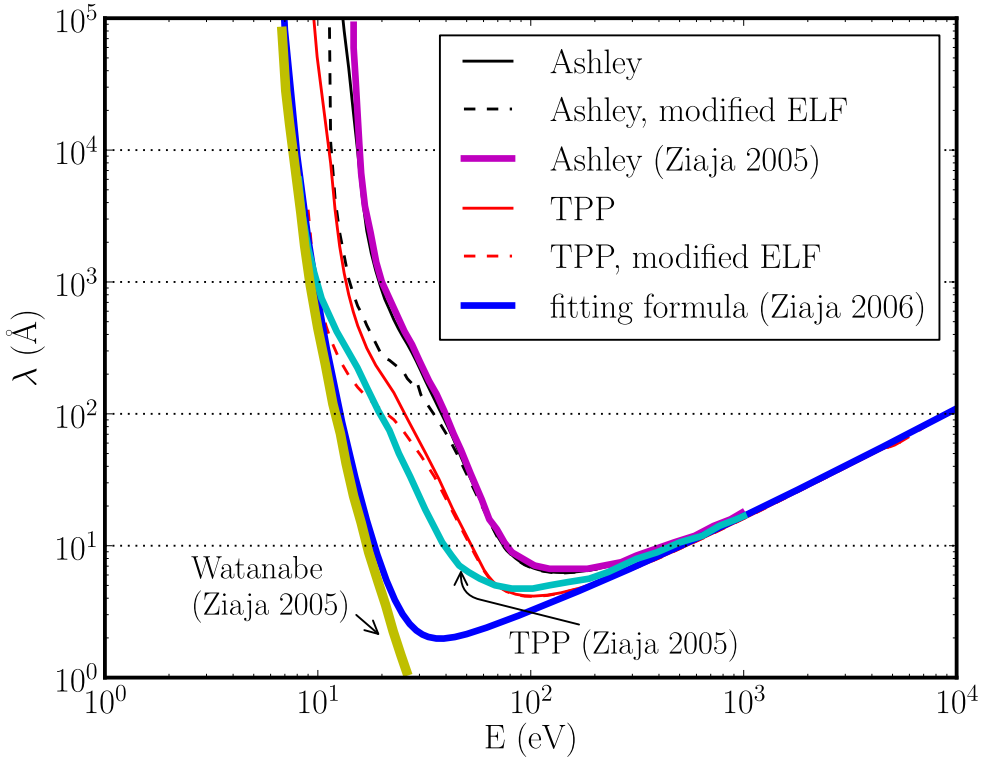
Energy loss functions used as input for the impact ionization calculations.

- The symbols are from published data (Philip & Taft 1964 for E < 35 eV; Ziaja *et al.* 2005 for E > 35 eV).
- The modified ELF at low E is for investigation of the sensitivity of the IMFPs on the low energy ELF.



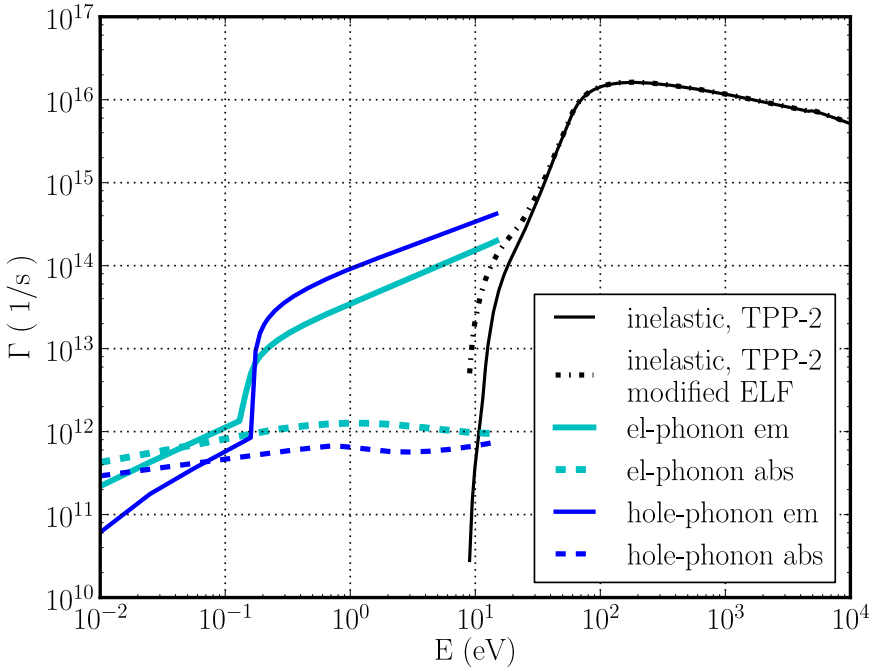
Calculated Inelastic Mean Free Paths (IMFPs) agree with results from a previous implementation.

- We compared our IMFPs to results from Ziaja *et al.* (2005-6), experimental data for E > 300 eV and band structure calculations at low E.
- The TPP model is in better agreement with band structure data at low E than the Ashley model.
- The optical models are in agreement for E > 300 eV.
- The only input to these models is the energy loss function (ELF) determined from optical experiments



Scattering with phonons is needed to model charge transport in diamond

- We implemented models from Jacoboni & L. Reggiani, Rev. Mod. Phys. (1983) for both electron-phonon and hole-phonon scattering.
- Emission and absorption of phonons are predominant at low energy (E < 10 eV).
- Impact ionization dominates high energy scattering, E > 50 eV.
- Our algorithm automatically switches electrons and holes from impact ionization to phonon scattering using an empirical rule.

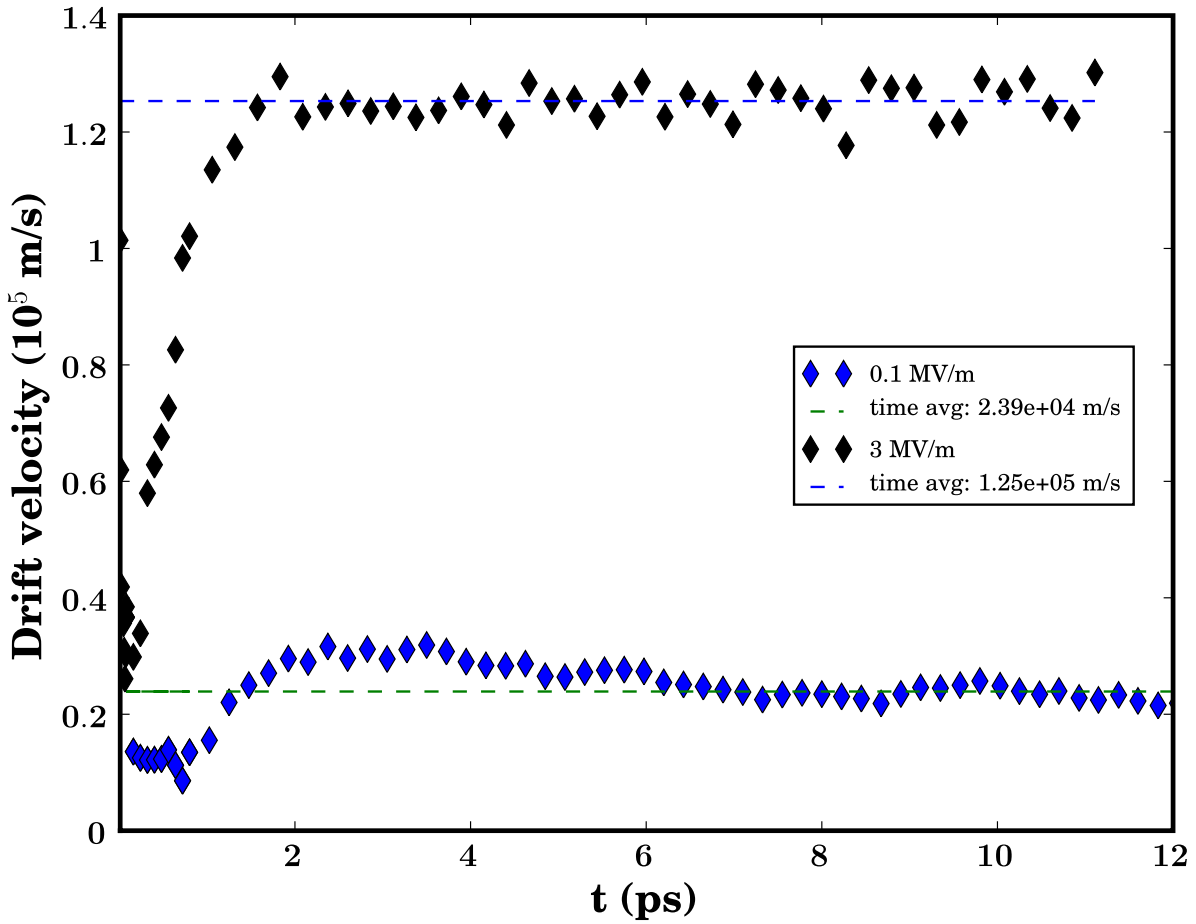


We implemented the following types of electron-phonon and hole-phonon scattering.

- Electron intra-valley *inelastic* scattering with acoustic phonons:
  - emission & absorption of phonons with energies (for diamond) in the range $0 < E_{phonon} < 0.12$ eV
- Electron inter-valley scattering is simulated with three different phonons with energies:
  - 0.16 eV (LO, g3 mode, between parallel valley); 0.13 eV (LA, f2 mode); 0.15 eV (TO, f3 mode)
  - The f# modes are for scattering between perpendicular valleys
- For hole-phonon scattering, we implemented a one-band model for heavy holes that includes:
  - intraband scattering with acoustic phonons
  - intraband scattering with optical phonons (0.17 eV).

The phonon models allow us to explore the drift state in applied electric field.

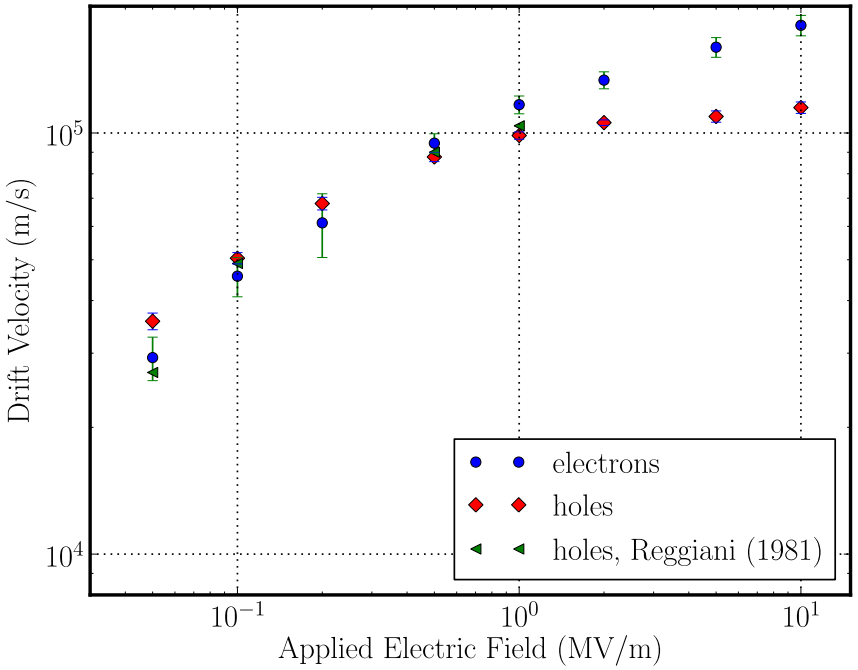
- As expected, the drift state is reached faster when increasing the applied field.



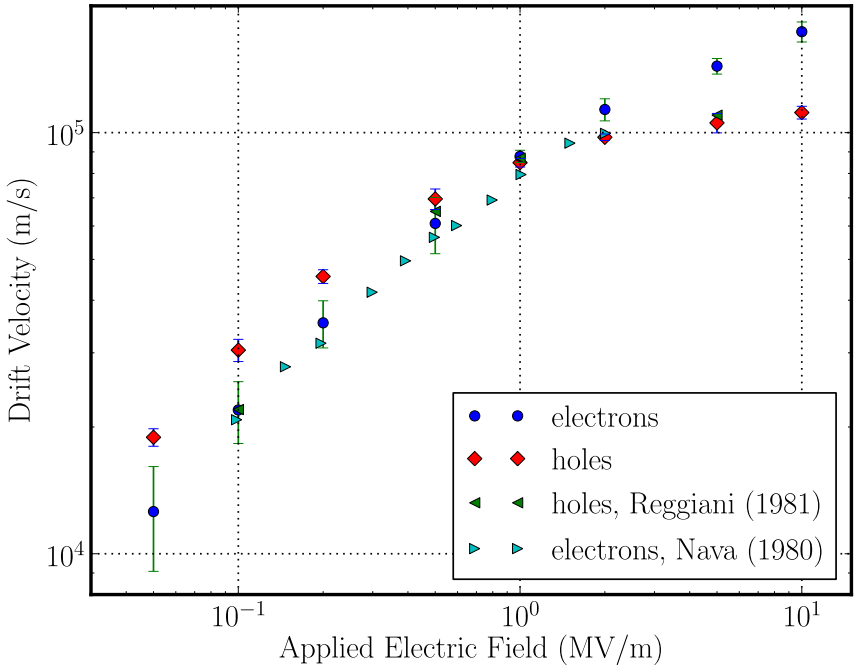
Drift velocities obtained with the phonon models show agreement with previous data.

- Temperature dependence and comparison to available data for drift velocities of electrons and holes:

150 K



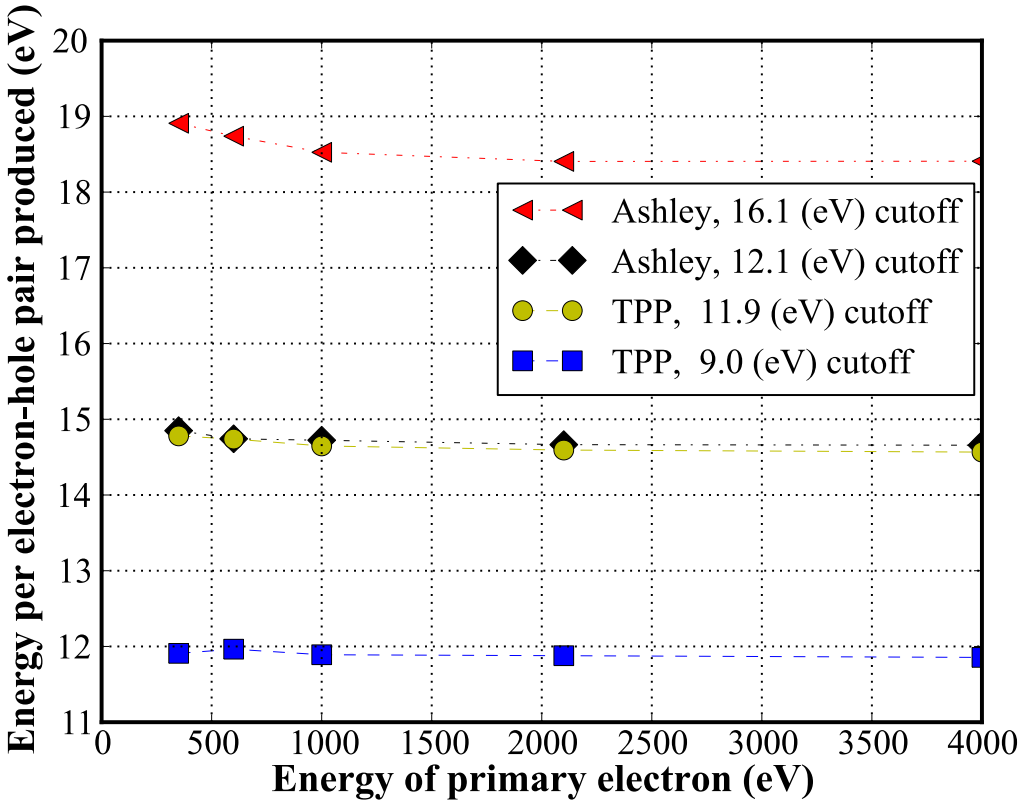
300 K



VORPAL provides results on the average energy to generate an electron-hole pair

- Results from from different models for impact ionization – the TPP model shows better agreement with experimental data.

- Our results agree with previous simulations (Ziaja *et al.* 2005 & 2006).
- The values from the TPP model are within ~10 % of recent experimental data but depend on the cutoff energy for switching to phonon scattering.



Comparison with previous results on the average energy to generate an el.-hole pair.

- Initial model (Klein, 1968) estimates it as function of the gap energy and the characteristic optical phonon energy via:

$$\epsilon = (14/5)\, E_g + r\hbar\omega_R$$

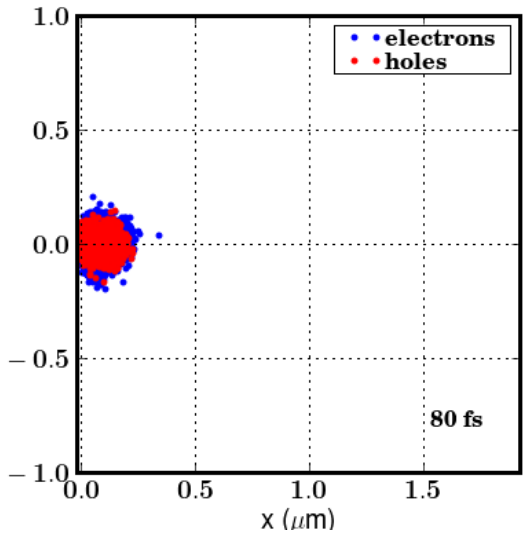
- However, it predicts about 17 eV which is markedly higher than recent experimental measurements that are in the range from 12.8 to 13.8 eV.
- Results have been reported (including experimental theoretical, and computational studies) that range from 9.8 eV to 17 eV.
- Our result with the TPP model and the 11.9 eV cutoff are within 10 % of the most recent 13.5 eV measurements.

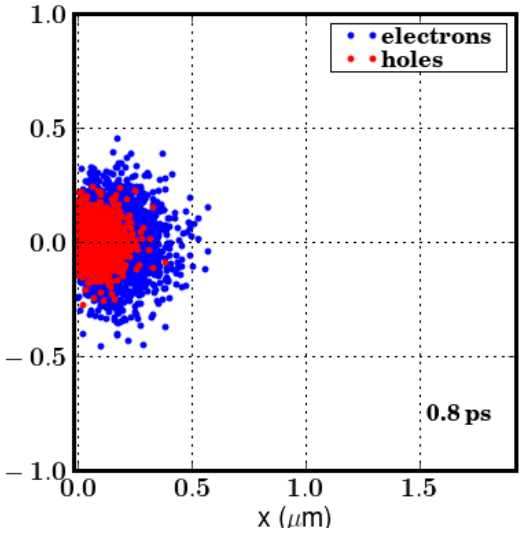
Simulation parameters for modeling transmission mode experiments

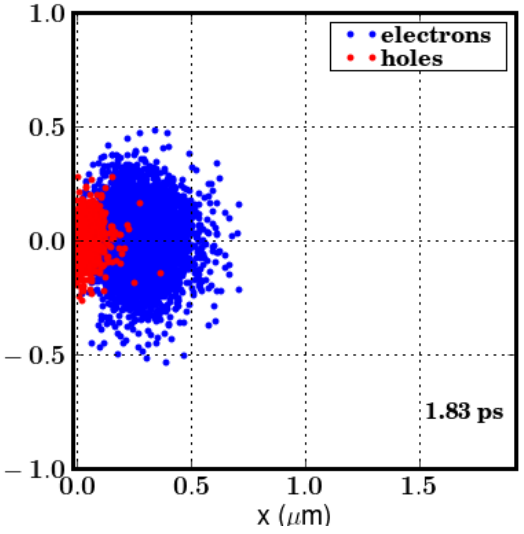
- Primary electrons enter the 3D simulation box with an initial velocity along the positive x-axis from the x=0 surface side at t = 0 s.
- The whole simulation box represents diamond at 300 K.
- Primary electrons create electron-hole (e-h) pairs in high energy inelastic scattering processes.
- Sufficiently energetic secondary electrons and holes (with energies higher than the energy gap E_G = 5.47 eV in diamond) also undergo such inelastic processes and thus generate additional e-h pairs.
- The e-h pair generation is essentially complete in a few 100 fs.
- Electrons and holes are switched to use a phonon scattering model when their energy becomes less than 11.9 eV within the first 400 fs.
- The metal contact at the x = 0 surface was modeled with a sink boundary condition – all particles moving to a position with x < 0 in a time step were removed from the simulation.

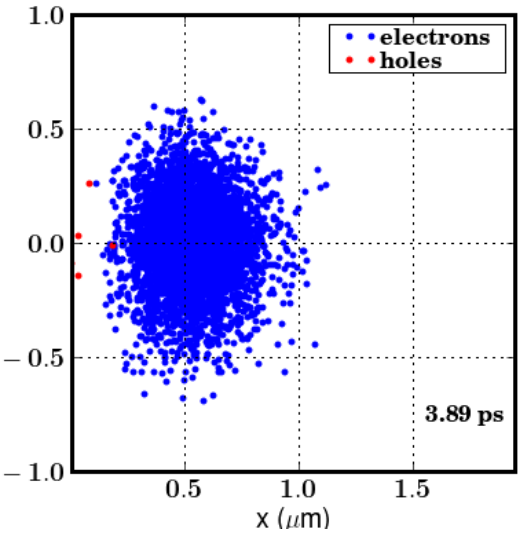
Evolution of electrons and holes generated from primary electrons

- The data is for 2.7 keV primary electrons in 3 MV/m applied field.



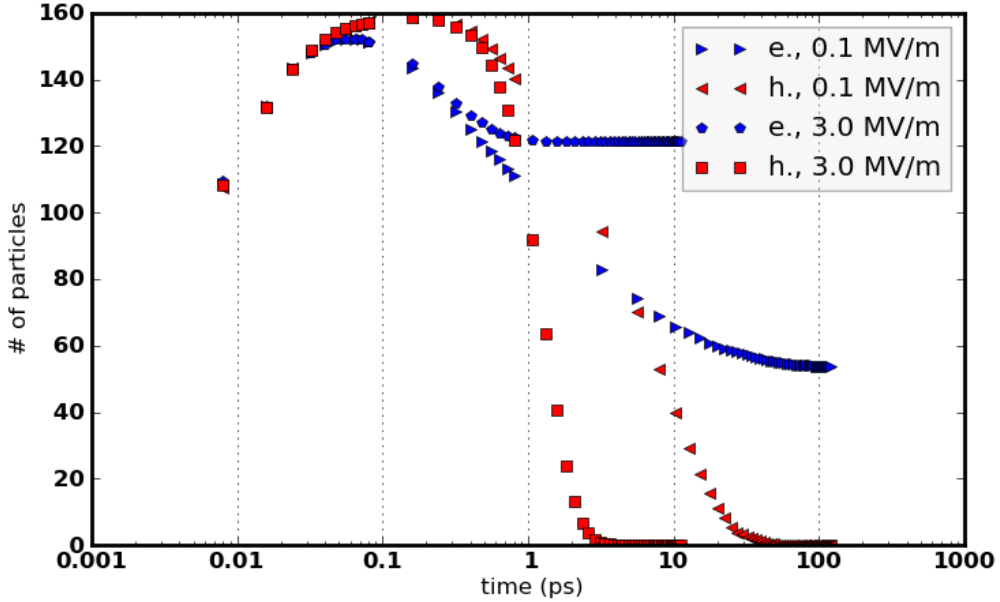






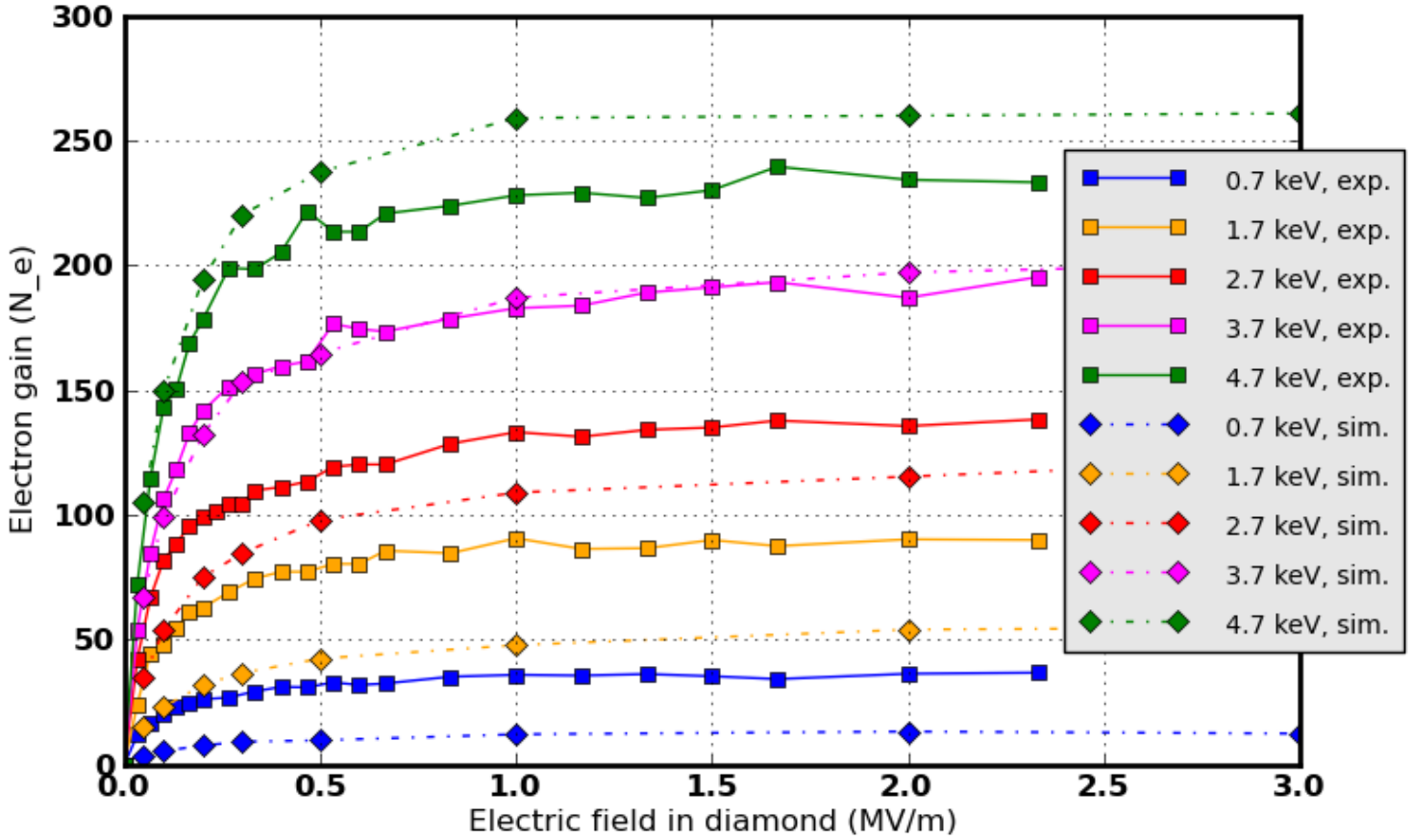
How do we determine electron gain from the simulations data?

- We estimate electron gain by counting the number of free electrons that drift away from the metal contact surface at x=0.
- The higher rate of phonon emission for holes is slowing down the hole cloud expansion and likely leading to the smaller loss of holes compared to electrons at earlier times (< 1 ps).



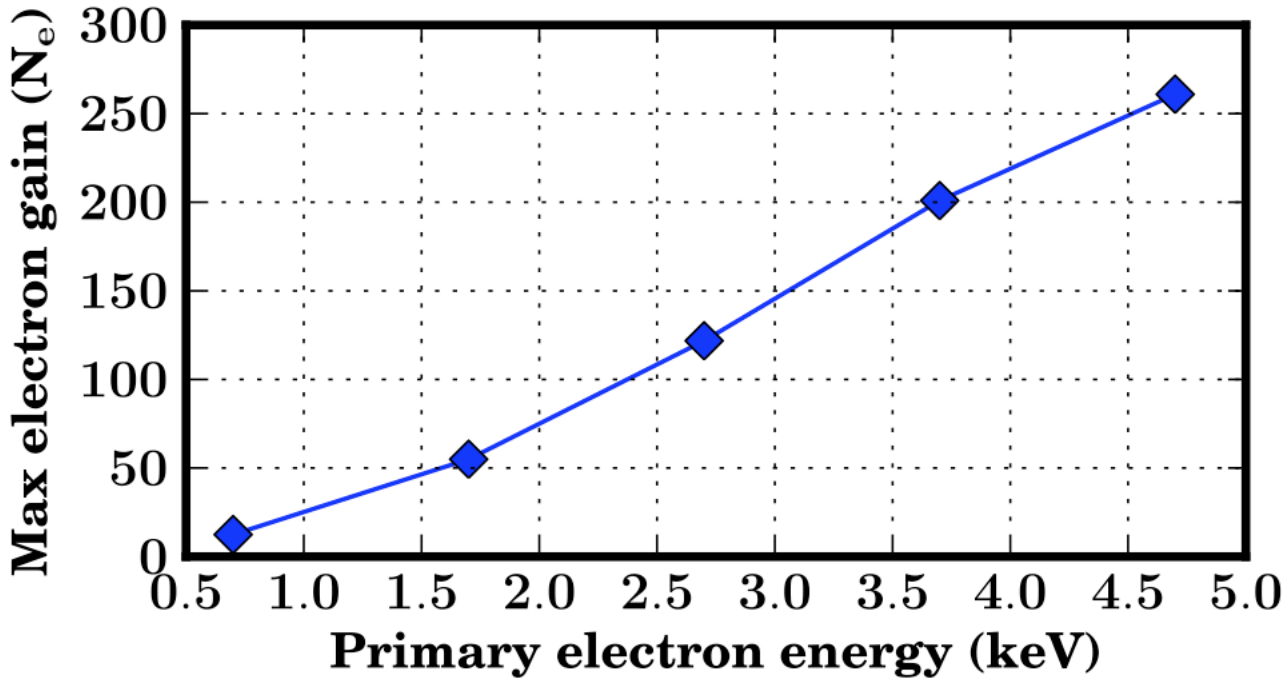
Comparison to experimental data

- Simulated electron gain shows overall qualitative agreement with the gain measured in transmission mode experiments.



Over two orders of magnitude charge gain can be achieved.

- Both the transmission mode experiments and the simulations indicate that two orders of magnitude charge gain for primary electron energy higher than 2.5 keV.



- We are considering to implement a model for the energy loss of primary electrons in the metal contacts (due to inelastic scattering) to better understand the experimental data.

What factors are affecting the observed level of agreement?

- The simulations do not take into account impact ionization and phonon scattering at the same time.
- The impact ionization model cannot be considered accurate for energies lower than 50 eV.
- Currently, the energy loss of primary electrons when going through the metal contacts is considered constant while it varies with the energy of the primaries, the kinds of metals used, and the thickness of the metal contact.
- Nevertheless, for primary energies from 2.7 keV to 4.7 keV, the agreement is close to 10 % at gain saturation fields.

We recently developed initial capabilities for electron emission simulations.

- Electron emission from diamond was recently demonstrated in emission-mode experiments (X. Chang *et al.*, accepted for publication in the Phys. Rev. Lett. 2010).
- We are developing new VORPAL code capabilities to enable simulation of electron emission from diamond.
- These simulations rely on a new feedback algorithm in VORPAL that allows a specified potential across a diamond-vacuum system to be established and maintained.
- The current code infrastructure we have developed allows us to:
  - model reflection of charge carriers at a diamond-vacuum interface
  - testing of electron emission using a constant probability rate

Initial approach to model emission from diamond with NEA & PEA

- For the surface potential, we are implementing the simple case of a potential step at the diamond-vacuum interface (the $x = 0$ plane):
  - in diamond: $V(x, y, z) = 0, x < 0$ and vacuum: $V(x, y, z) = \chi, x \geq 0$
  - PEA is modeled with: $\chi > 0$ and NEA with: $\chi < 0$
- The probability for emission of an electron with energy E impacting the diamond surface at an angle α to its normal is:

$$P(E, \alpha) = \frac{4\sqrt{1 - \frac{\chi}{E\cos^2(\alpha)}}}{\left(1 + \sqrt{1 - \frac{\chi}{E\cos^2(\alpha)}}\right)^2}$$

- The change of the direction of propagation of the emitted electron is:

$$\sin\beta = \sqrt{\frac{E}{E - \chi}}\sin\alpha$$

and its momentum amplitude: $\sqrt{2m_e(E - \chi)}$

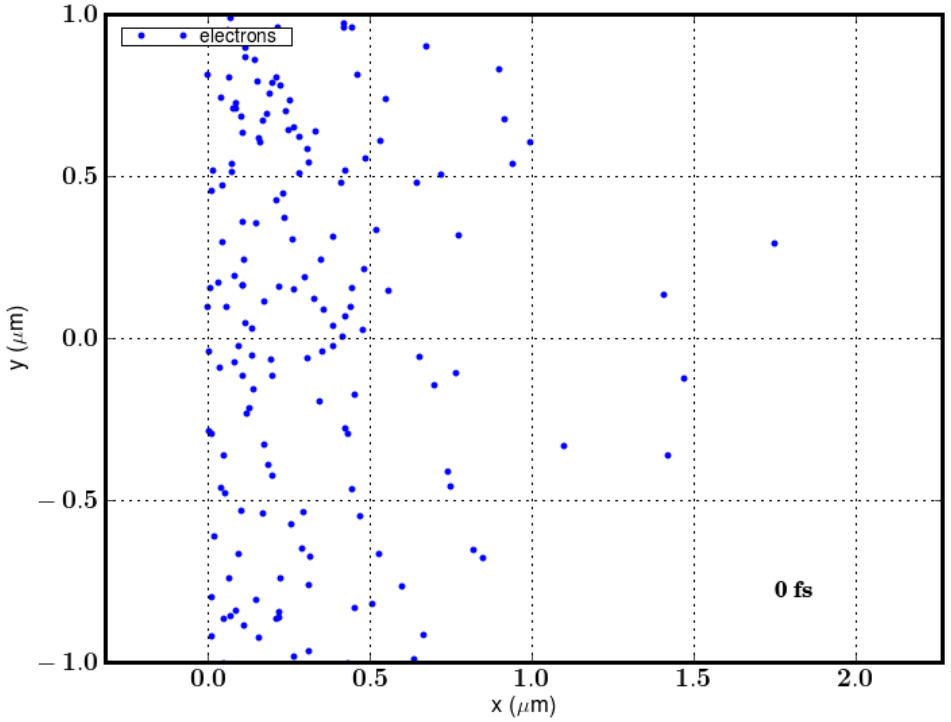
- Note that this model does not take into account the different effective masses of the electron in diamond and vacuum.

Initial approach for modeling collection efficiency of diamond x-ray detectors.

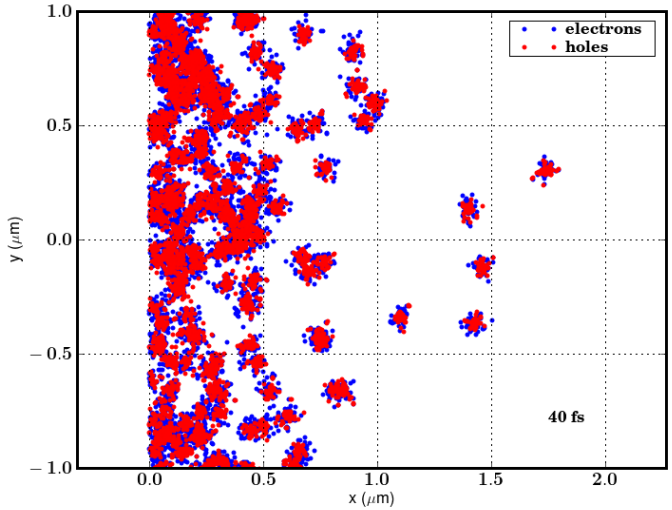
- Simulation parameters are similar to those for the transmission mode simulations.
- Instead of high-energy electrons, x-ray photons are initiating the generation of electron-hole pairs.
- Each absorbed photon transfers its energy to create a high-energy electron and a hole.
- The location of the initial electron-hole pairs are given by the distribution expected from attenuation of light in diamond.
- The photon absorption probability distribution exponentially decreases with depth.

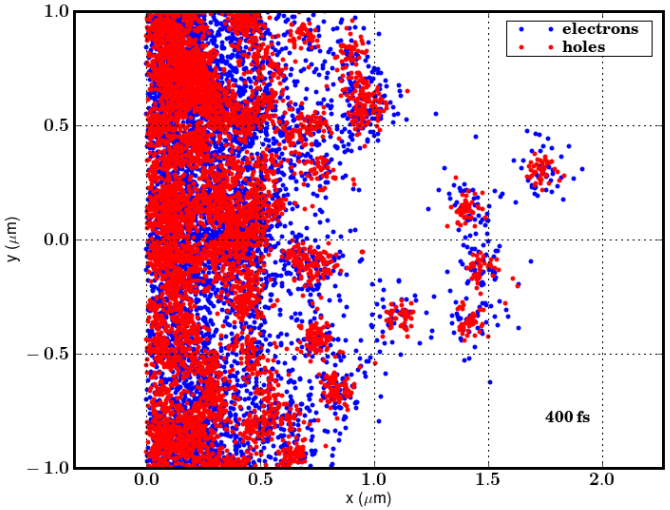
The detector simulations are started with a distribution of electron-hole pairs.

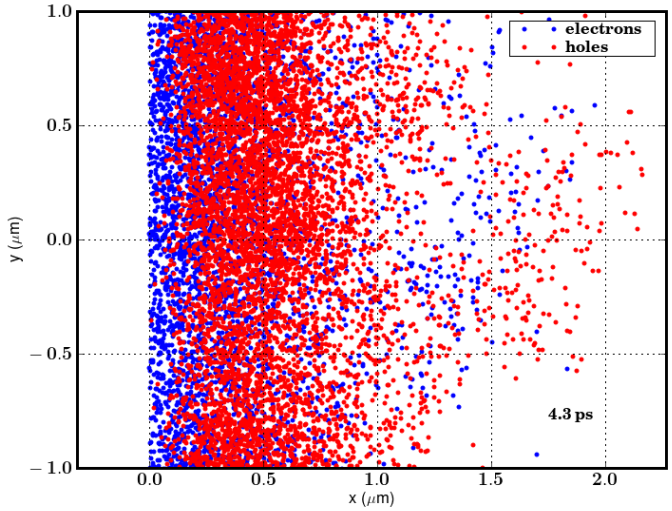
- The simulation parameters are identical to single particle transmission-mode simulations, except for:
  - multiple electron-hole pairs were distributed
  - transverse size was varied along with longitudinal size, depending on the total drift before entering a steady state
  - note that these particle plots show particles from four simulations

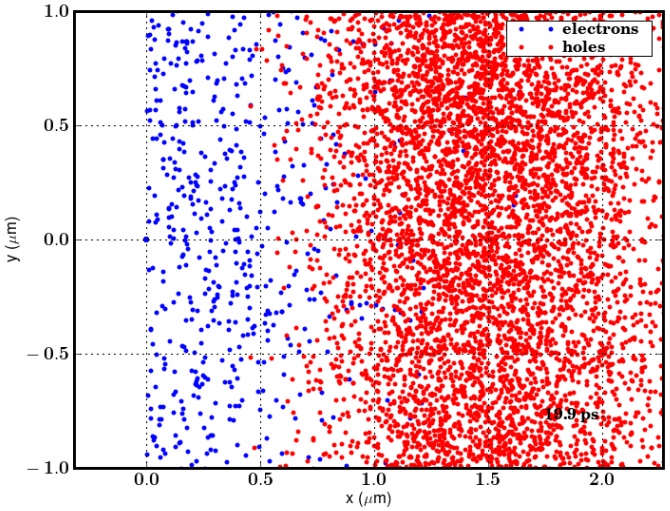


Electron and hole evolution in detector simulations gives the time scale for separation.



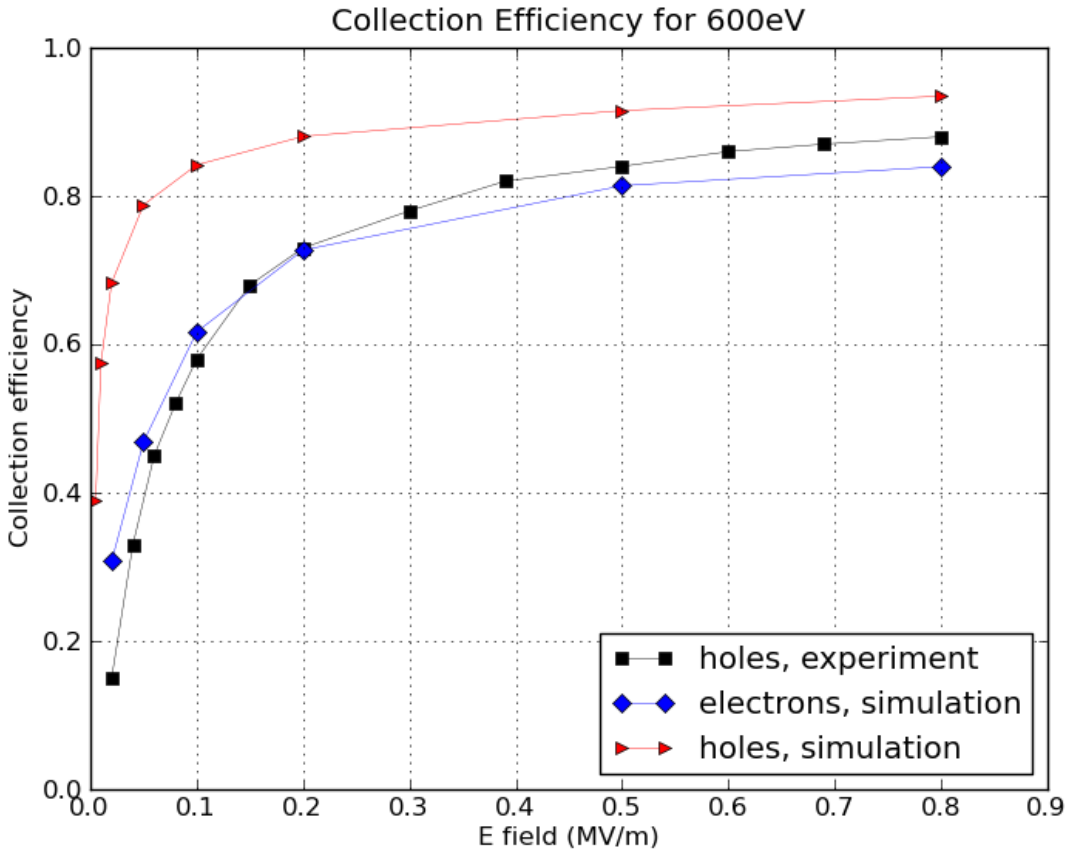






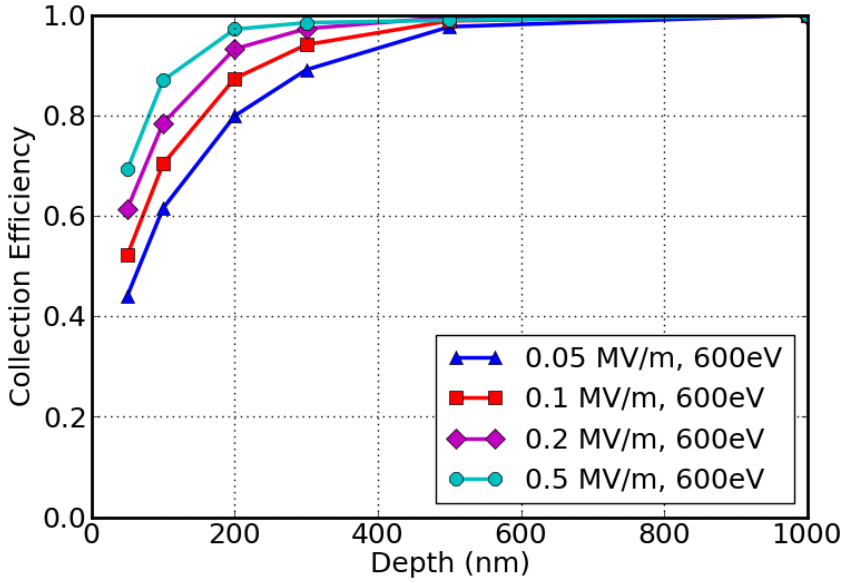
How do we determine collection efficiency from the simulation data?

- Collection efficiency is determined by the ratio of electrons separated from the surface over the total number of electrons that would be created in bulk diamond
- The electron gain in the bulk is simulated in separate simulation
- Collection efficiency has also been measured and simulated for holes.

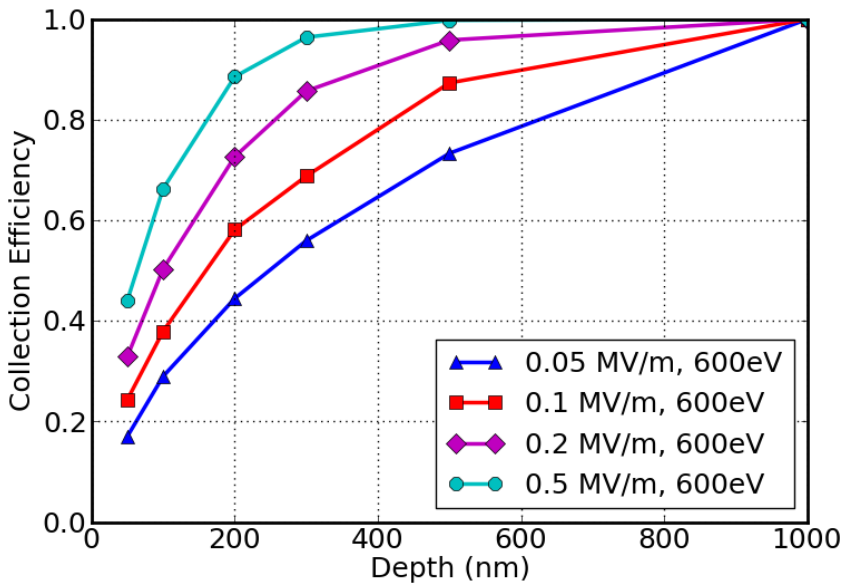


Simulations allow us to directly investigate collection efficiency (CE) vs depth.

- We have also run simulations with single particles at varying depth
- The dependence of the obtained collection efficiency (shown here for 600 eV photons) vs absorption depth and applied electric field shows higher CE for holes vs electrons.
- This is likely due to the higher phonon scattering rates.



CE of holes



CE of electrons

VORPAL simulations provide a realistic explanation of the observed CE data.

- Simulations data on CE vs depth and applied field was used to formulate a model for the observed responsivity:

$$S(\nu) = \frac{1}{W_C} \exp\left(-\frac{t_M}{\lambda_M(\nu)}\right)\left(1 - \exp\left(-\frac{t_C}{\lambda_C(\nu)}\right)\right) CE(\nu, E)$$

- This expression takes into account the loss of charge to the incident metal contacts due to diffusive motion.
- It provides a physical description of the observed data over different applied fields and photon energies (J. W. Keister, J. Smedley, D. A. Dimitrov, and R. Busby, *Charge Collection and Propagation in Diamond X-ray Deterctors*, IEEE Transactions on Nuclear Science, **57**, 2400 (2010)).

Summary

- The currently implemented models for diamond allow us to investigate:
  - Secondary electron and hole generation
  - Relaxation of the electrons to the drift state due to scattering with phonons and charge transport
  - Space-charge effects (since VORPAL solves Maxwell's equations)
- VORPAL simulation results using these models have allowed better understanding of:
  - transmission-mode diamond-amplifier experiments
  - collection efficiency measurements for investigation of diamond detectors
- These models and simulation results are described in: D. A. Dimitrov, R. Busby, J. R. Cary, I. Ben-Zvi, T. Rao, J. Smedley, X. Chang, J. Keister, Q. Wu, E. Muller, *Multiscale 3D simulations of charge gain and transport in diamond*, to appear in J. App. Phys. (2010).
- We are currently implementing models for electron emission from diamond with different electron affinities.
- We are also considering the implementation of models for electron and hole trapping, and different types of diamond-metal contacts.