New VORPAL Modeling Capabilities for 3D Multiscale Simulations of Charge Gain and Transport in Diamond Devices

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Outline

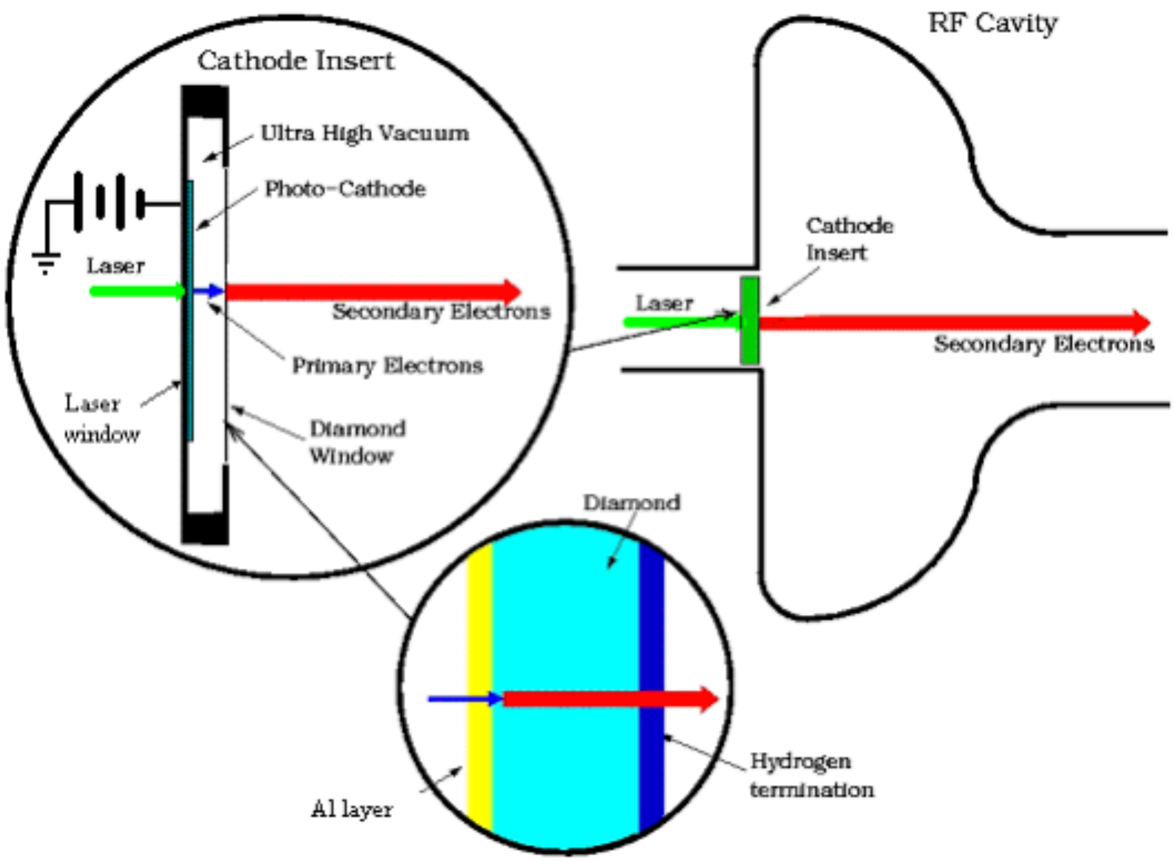
- Motivation
  - Diamond-amplifier cathode concept & types of experiments
  - Diamond-based beam line detectors
- Models developed in VORPAL to simulate diamond amplifier & detector physics:
  - Secondary electron generation
  - Electron-phonon and hole-phonon scattering for simulation of charge transport, charge impurity scattering
  - 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
- Results
- 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

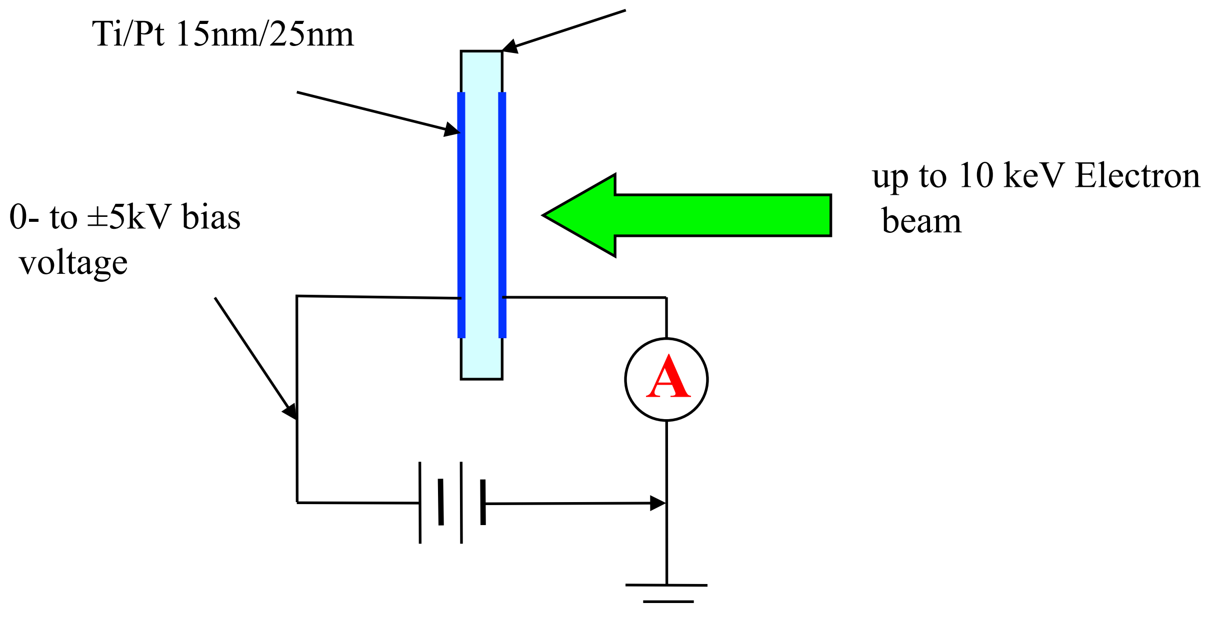
- The overall concept includes:
  - a drive laser for primary electrons
  - a diamond sample for electron charge amplification
  - RF cavity for acceleration of electrons from the diamond emitters



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.



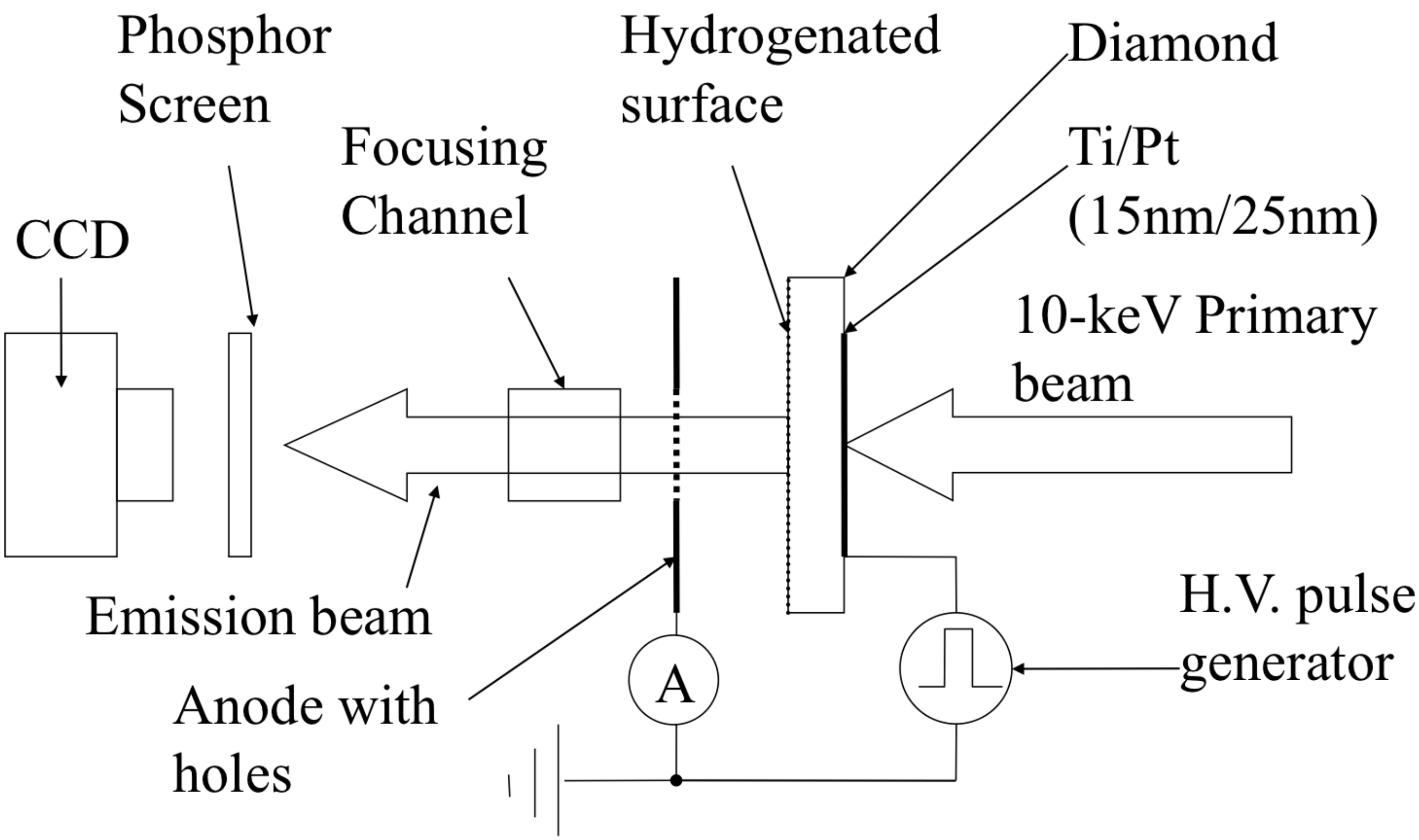
DC Transmission-mode Experiment

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.

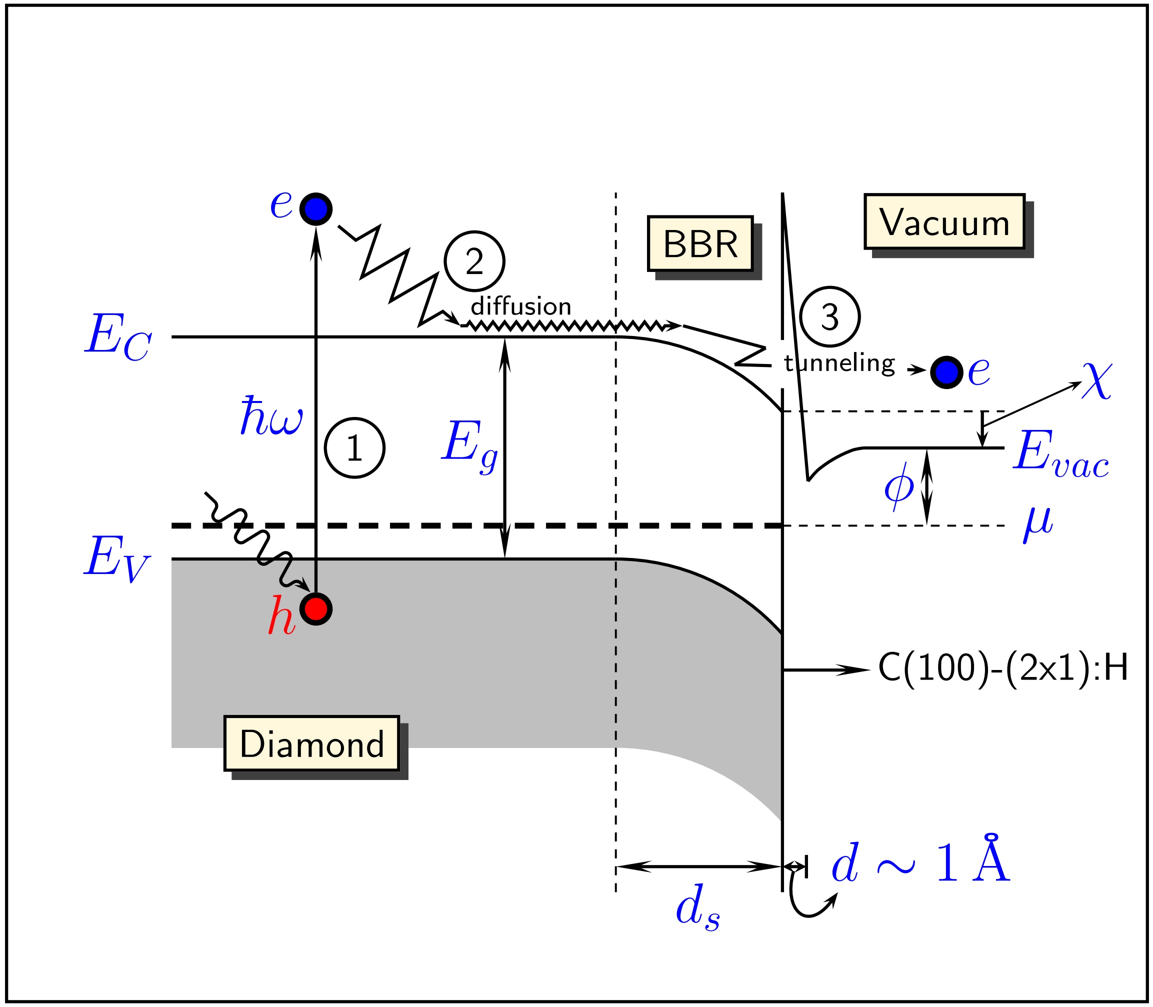
Electron emission from diamond was measured recently.

- 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.

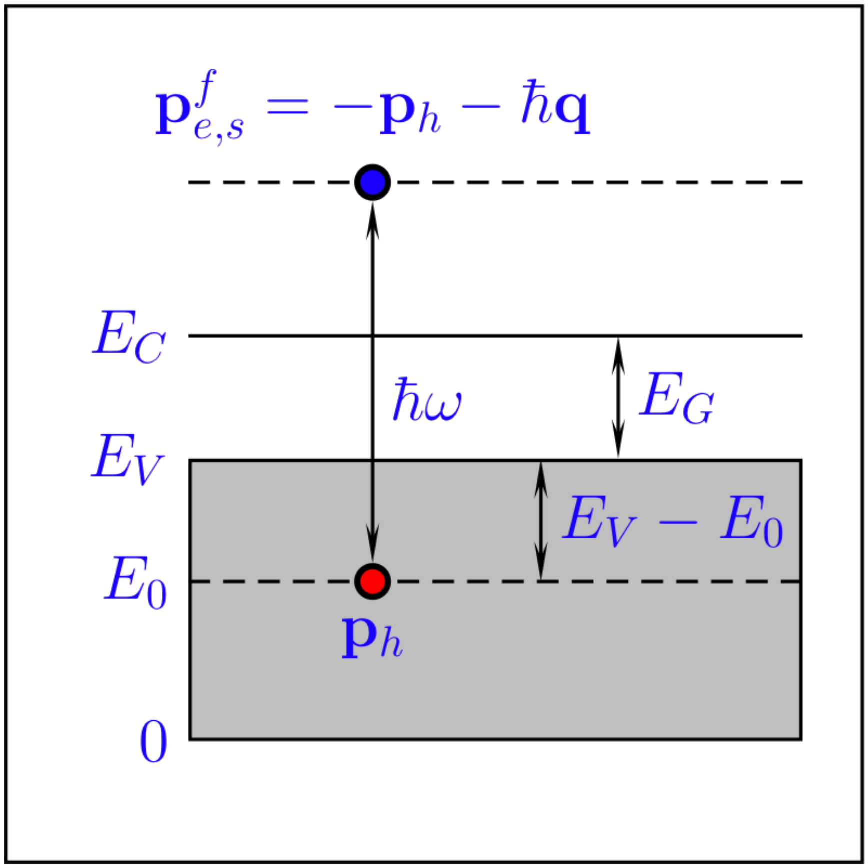
- To enable end-to-end simulations of diamond-amplified electron emitters we developed algorithms to model:
  - Inelastic scattering of electrons (primary & secondary) and holes for generation of electron-hole (e-h) pairs
  - Elastic scattering
    - at higher energies (> ~10 eV)
    - due to ionized 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:

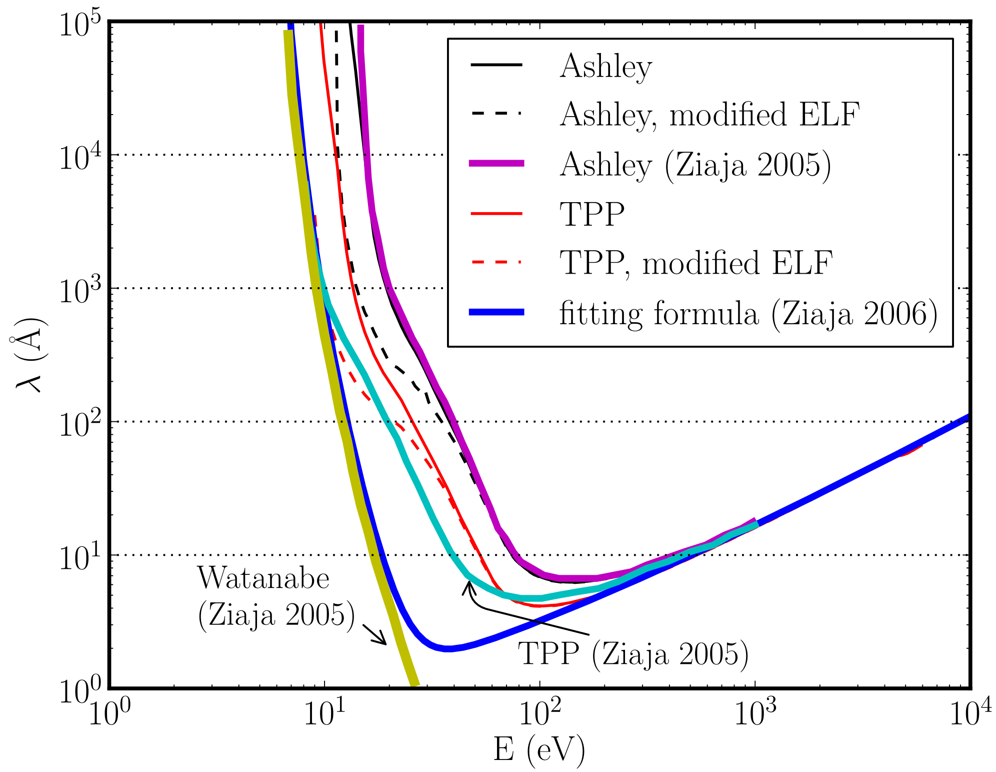
  Ziaja et al., Phys. Rev. B 2001 & 2002, and J. Appl. Phys. 2005.

- *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.



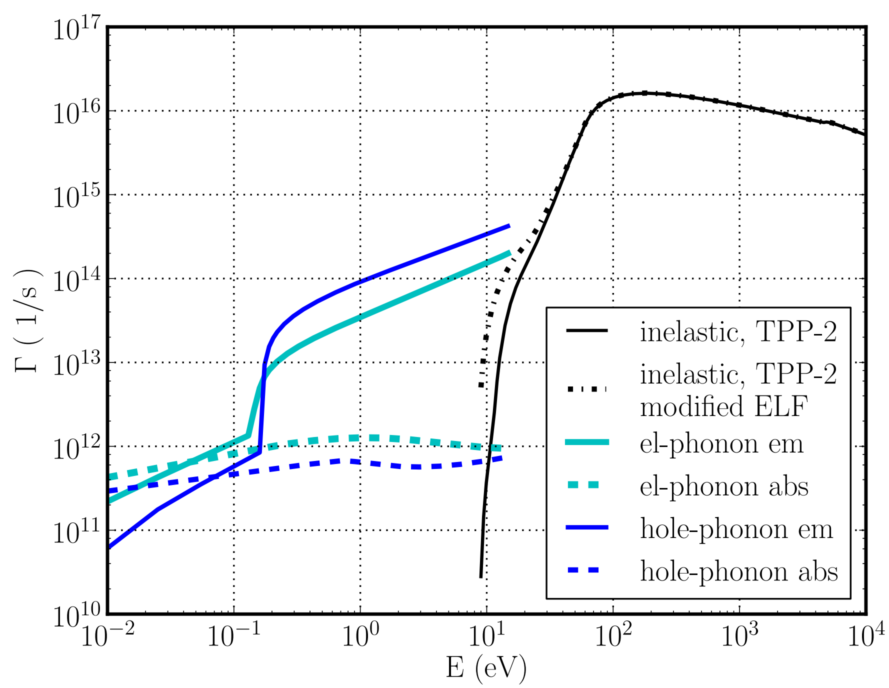
Calculated Inelastic Mean Free Paths (IMFPs) agree with results from a previous implementation.

- 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

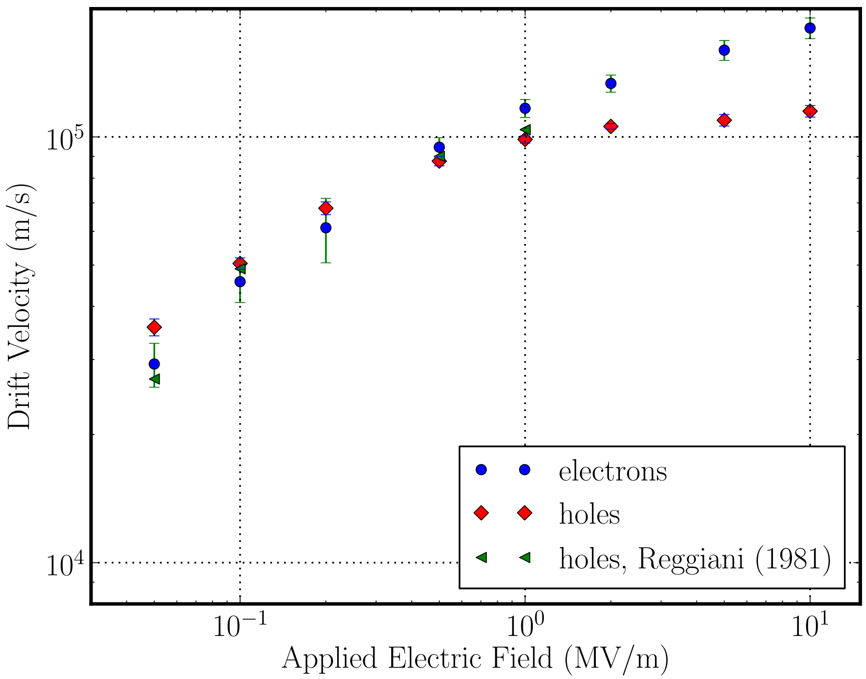
- We implemented models from Jacoboni & L. Reggiani, Rev. Mod. Phys. (1983) for both electron-phonon and hole-phonon scattering.
- Emission and absorption of phonons are predominant at low energy (E < 10 eV).
- Impact ionization dominates high energy scattering, E > 50 eV.
- Our algorithm automatically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



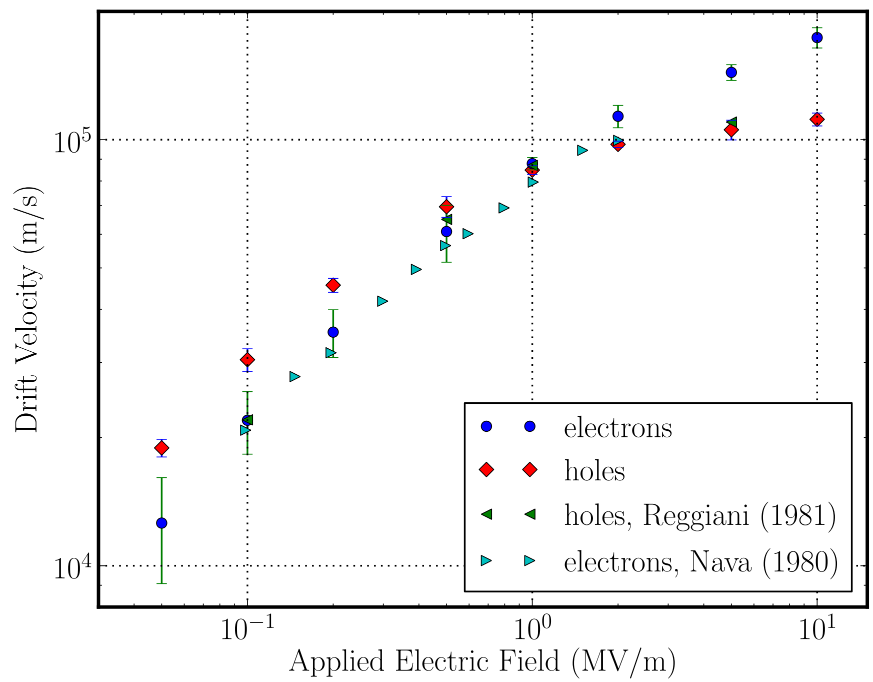
Drift velocities obtained with the phonon models show agreement with previous data.

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

150 K



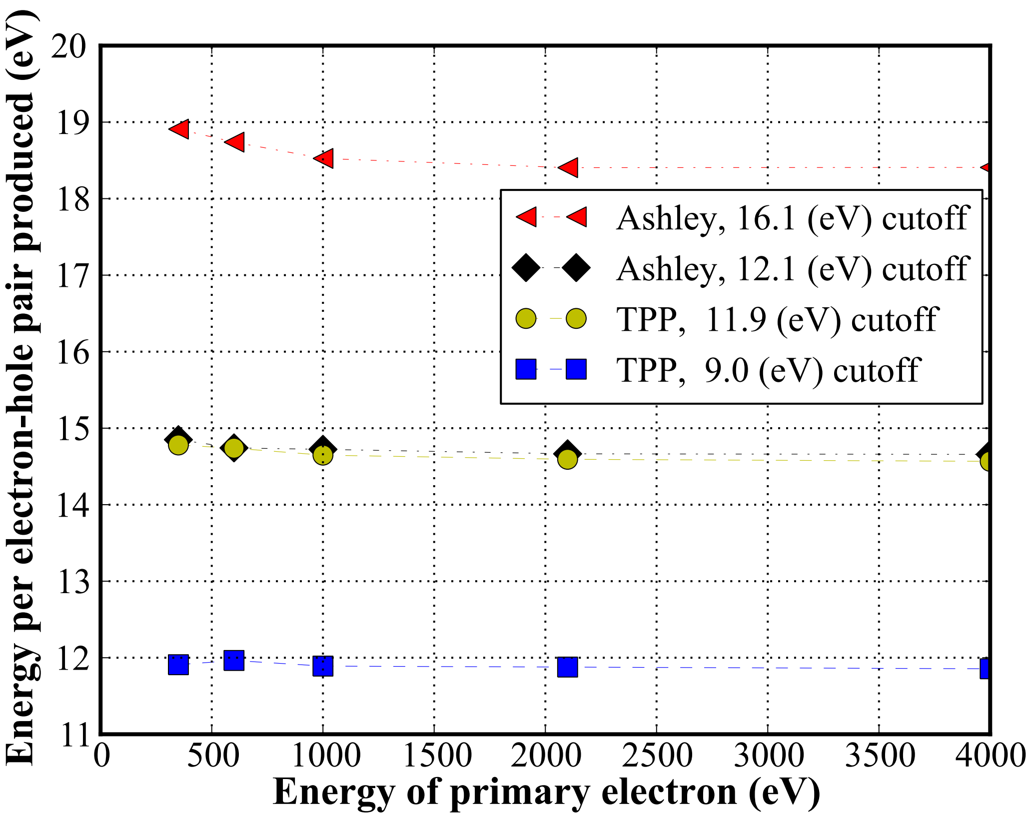
300 K



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:

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

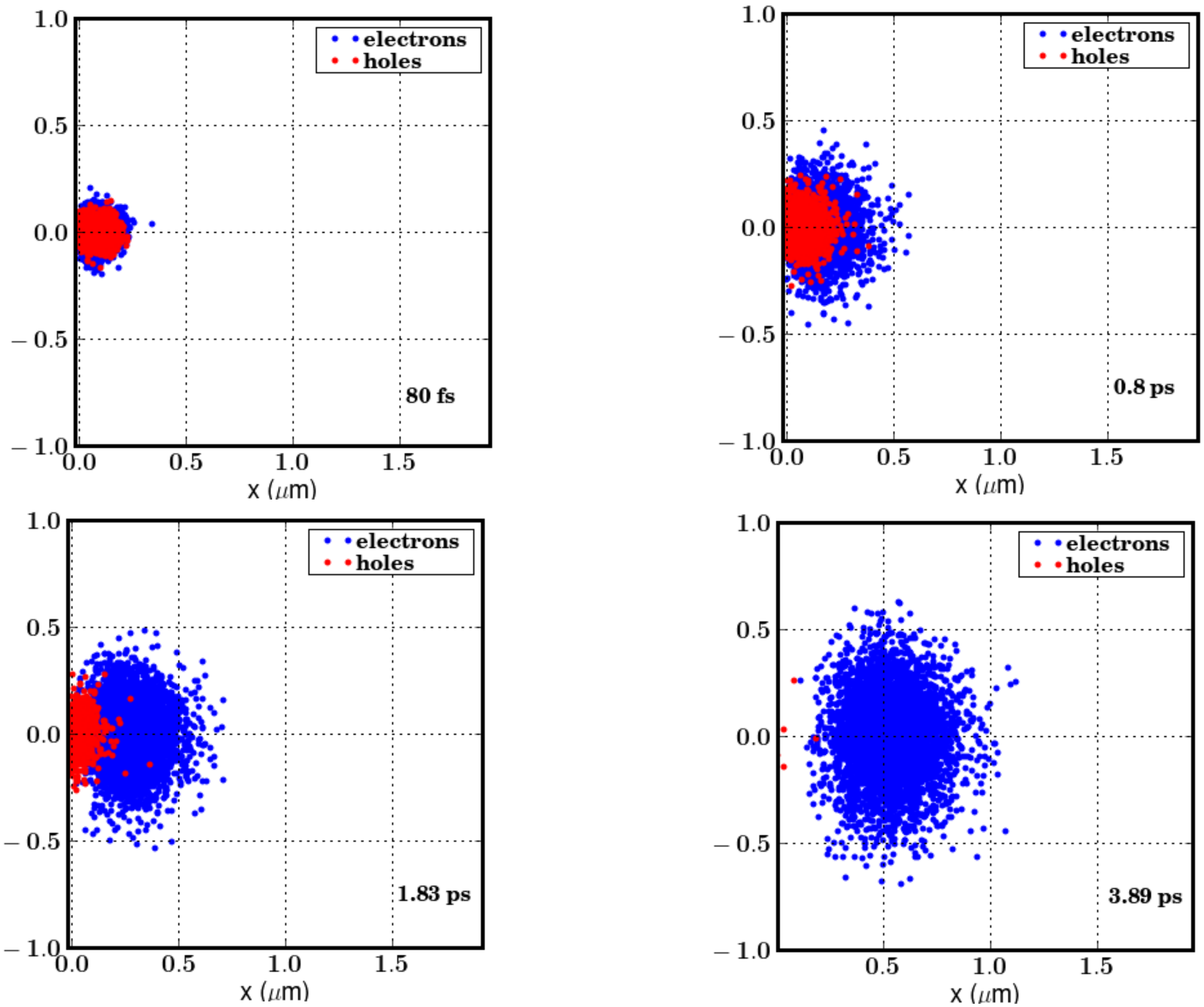
- However, it predicts about 17 eV which is markedly higher than recent experimental measurements that are in the range from 12.8 to 13.8 eV.
- Results have been reported (including experimental theoretical, and computational studies) that range from 9.8 eV to 17 eV.
- Our result with the TPP model and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

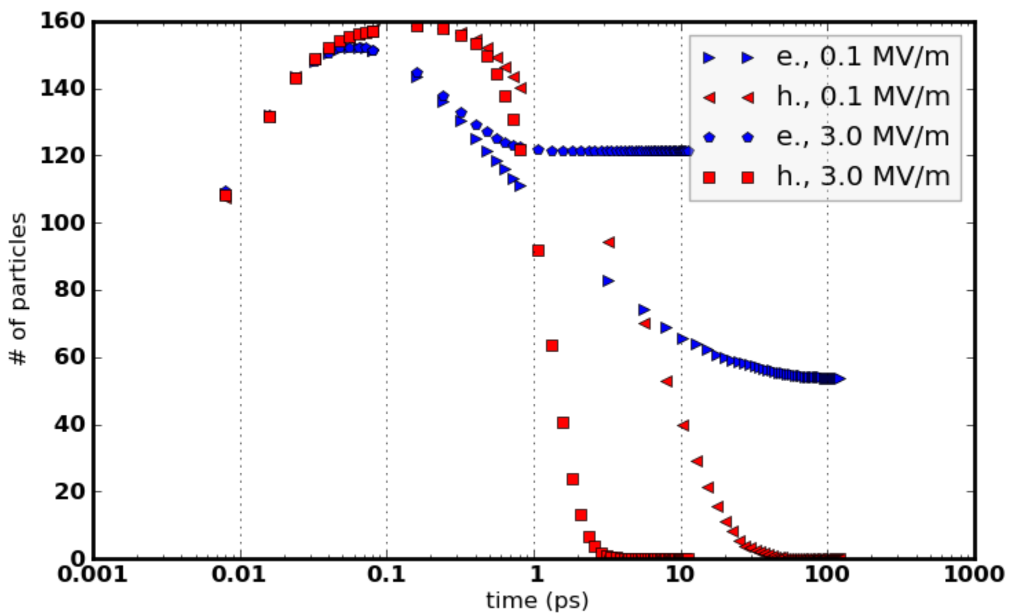
Evolution of electrons and holes generated from primary electrons

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



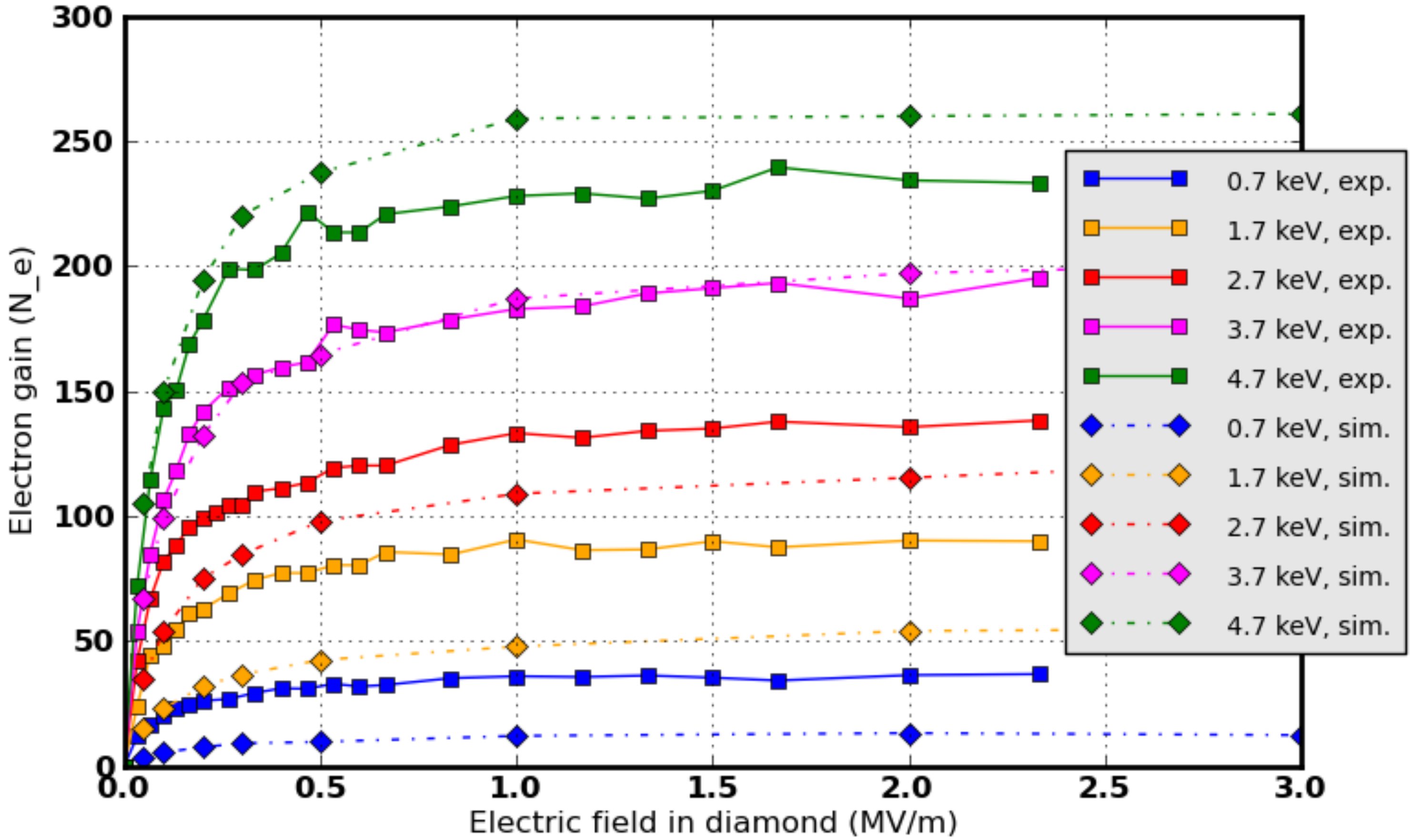
How do we determine electron gain from the simulations data?

- 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).



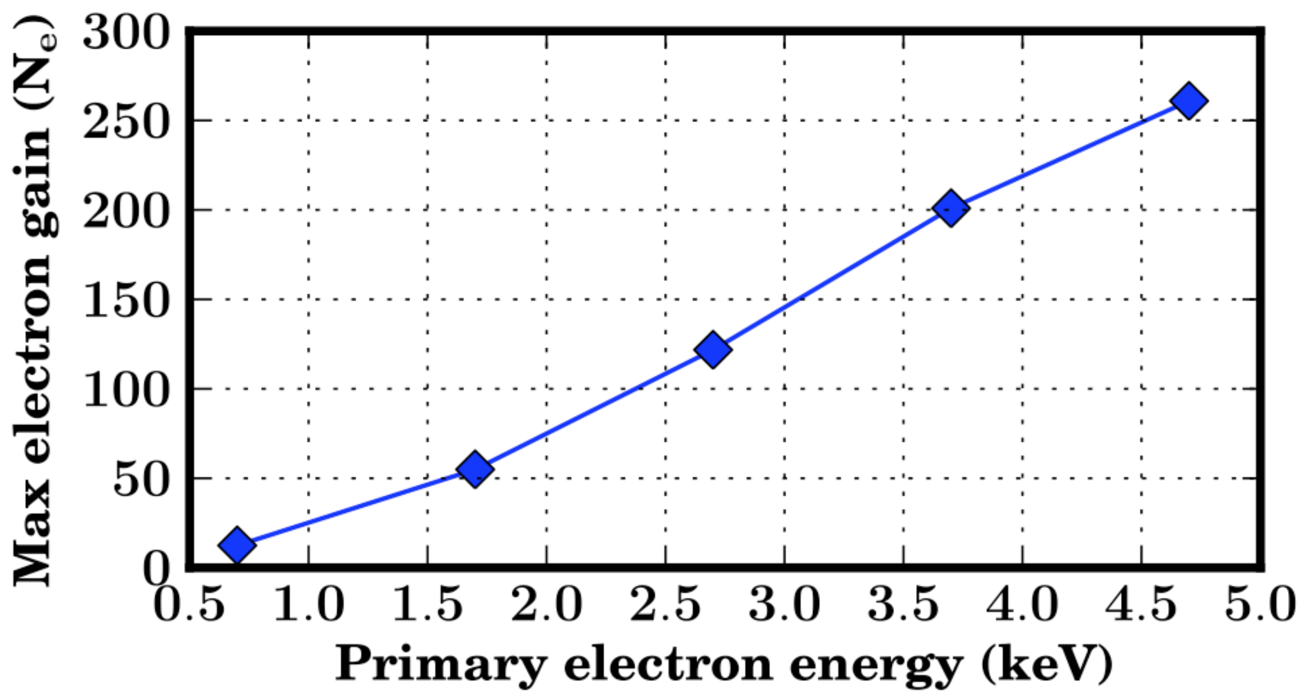
Comparison to experimental data

- 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.

We recently developed 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 Physical Review Letters).
- 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

Our work on this project was recognized in the peer-reviewed papers (2010).

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Summary

- The currently implemented models for diamond allow us to investigate:
  - Secondary electron and hole generation for different primary electron energies
  - Relaxation of the electrons to the drift state due to scattering with phonons and charge transport
  - The effects of fully taking into account the space-charge effects by solving Maxwell equations with VORPAL
- VORPAL simulation results using these models have allowed better understanding of transmission-mode and collection efficiency experiments conducted in BNL.
- We are currently considering the addition of detailed models for electron emission, trapping, electron affinity, and metal contacts.
- The new modeling capabilities developed under this SBIR project are being investigated for use in the aerospace industry.