Modeling Electron Emission From Diamond-Amplified Cathodes

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- Ivan Bazarov, Siddharth Karkare (Cornell University) and Jonathan Rameau (BNL) for useful discussions and suggestions,
- The VORPAL code developers for maintaining and extending its capabilities.

Outline

- Motivation
  - Diamond-amplifier cathode concept & experiments
  - Better understanding of electron emission data
- New electron emission models recently implemented in the VORPAL code
- Results
  - Verification of implemented models
  - Comparison of simulation results with experimental data from BNL on electron emission
- Summary

Motivation – Why should we develop simulation models for electron emission?

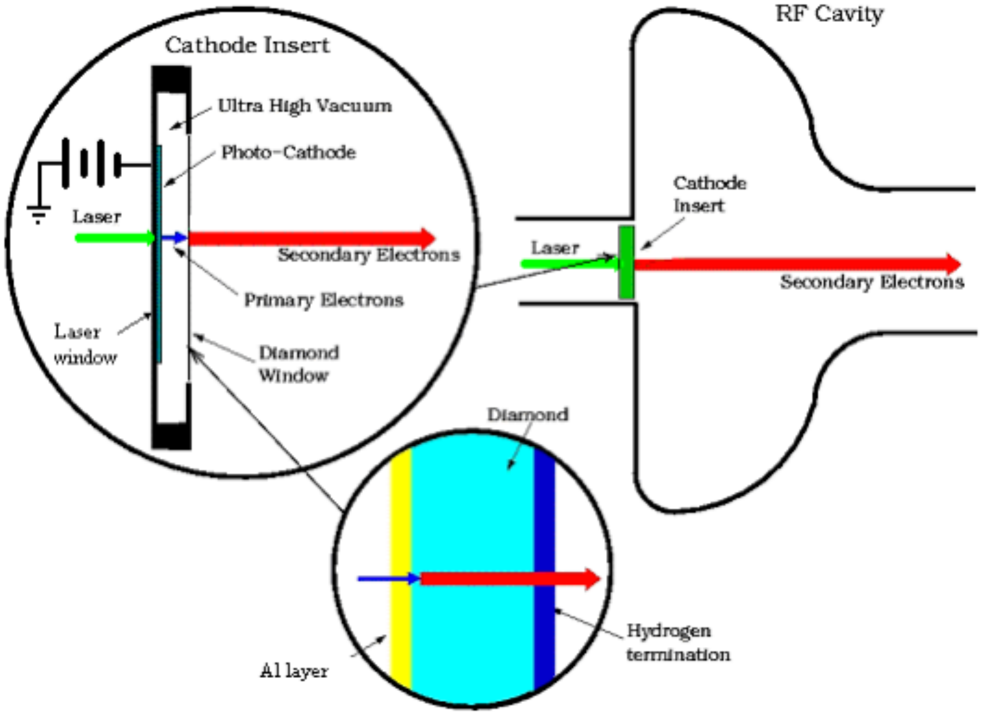
- A new diamond-amplified cathode was proposed to enable *high quantum efficiency* sources with *long lifetime*, *high-brightness*, and *low emittance* electron beams.
- Experiments have already demonstrated the potential of the concept. However, better understanding of the experimental data is needed to determine optimal designs for different applications.
- Simulations provide an efficient way to explore relevant parameter regimes to improve our understanding of electron emission and how to design cathodes with optimal physical properties.

Experiments have shown large variation of surface properties affecting emission.

- [*] J. B. Cui *et al.*, Phys. Rev. B **60**, 16135 (1999):
  - electron affinity was measured to vary from 0.38 eV (PEA) to -1.27 eV (NEA) for (111) diamond surface depending on hydrogenation coverage during preparation
  - surface graphitic patches were introduce to interpret the observed emission
- [**] F. Maier *et al.*, Phys. Rev. B **64**, 165411 (2001):
  - Experiments to measure electron affinity of (100) diamond surfaces showing variation from NEA of -1.3 eV to PEA of 1.7 eV.
- [#] E. Wang *et al.*, PRST-AB **14**, 111301 (2011):
  - Diamond-amplifier related experiments in BNL have shown decrease of electron emission over time due to charge accumulation at the emission surface – effective NEA introduced to interpret the data.
- [##] J. D. Rameau *et al.*, Phys. Rev. Lett. **106**, 137602 (2011):
  - NEA of up to -0.96 eV was measured from boron doped 100 diamond surfaces using angle resolved photoemission spectroscopy
  - Emission data were interpreted based on the Franck-Condon effect

Overall Diamond-Amplifier Cathode Concept

1. A drive laser pulse and a conventional photocathode are used to generated for primary electrons with keV energies.
2. The primary electrons enter a diamond slab, generate secondary electrons and holes that propagate in applied field to a negative electron affinity emission surface.
3. Amplified beam of secondary and primary electrons are emitted from diamond into an RF cavity.

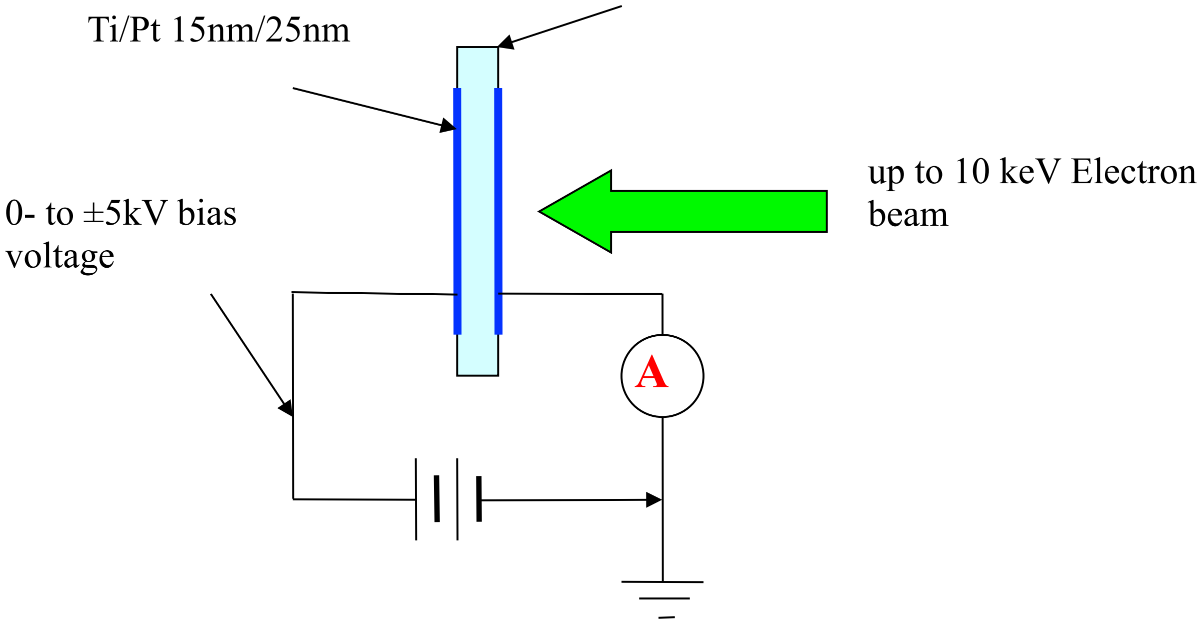


Schematic diagram of a secondary emission enhanced photoinjector (SEEP)

Diagram courtesy of Triveni Rao, BNL.

Probability of emission is measured using two types of experiments.

- First, the electron charge (using the transmitted current I_t) that could potentially be emitted from diamond is measured in transmission-mode experiments.
- Metal contacts are applied to opposite surfaces of diamond to apply an electric field inside, transport, and collect the generated charge carriers.



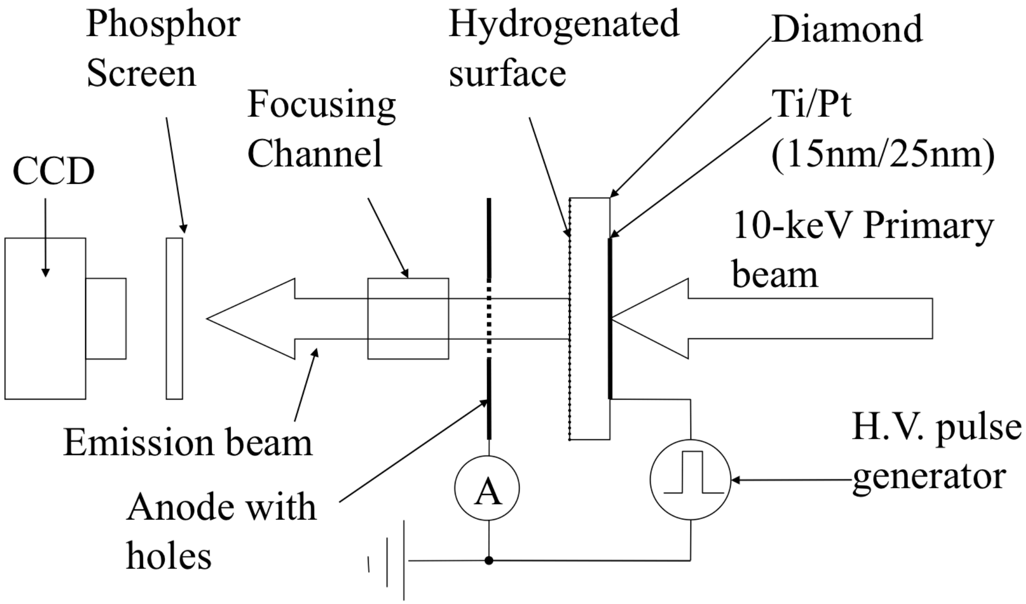
DC Transmission-mode Experiment
diagram courtesy of Xiangyun Chang, BNL

Emission-mode experiments measure the electrons collected in vacuum.

- Emission-mode experiments are designed to measure the electron current I_e collected in vacuum.
- The time-averaged probability of emission from the experimental data is defined as

$$P_e = I_e/I_t$$

- First emission experiments (X. Chang *et al.* Phys. Rev. Lett. **105**, 164801 (2010)) demonstrated a gain of 40 that was later improved to 178 - over two orders of magnitude (E. Wang *et al.*, PRST-AB **14**, 061302 (2011)).



Here, we consider simulations for modeling the probability of emission experimental data in [#].

- The experiments in [#] showed:
    - dependence of the probability of emission on applied field
    - variation of observed values due to measurements from different diamond samples

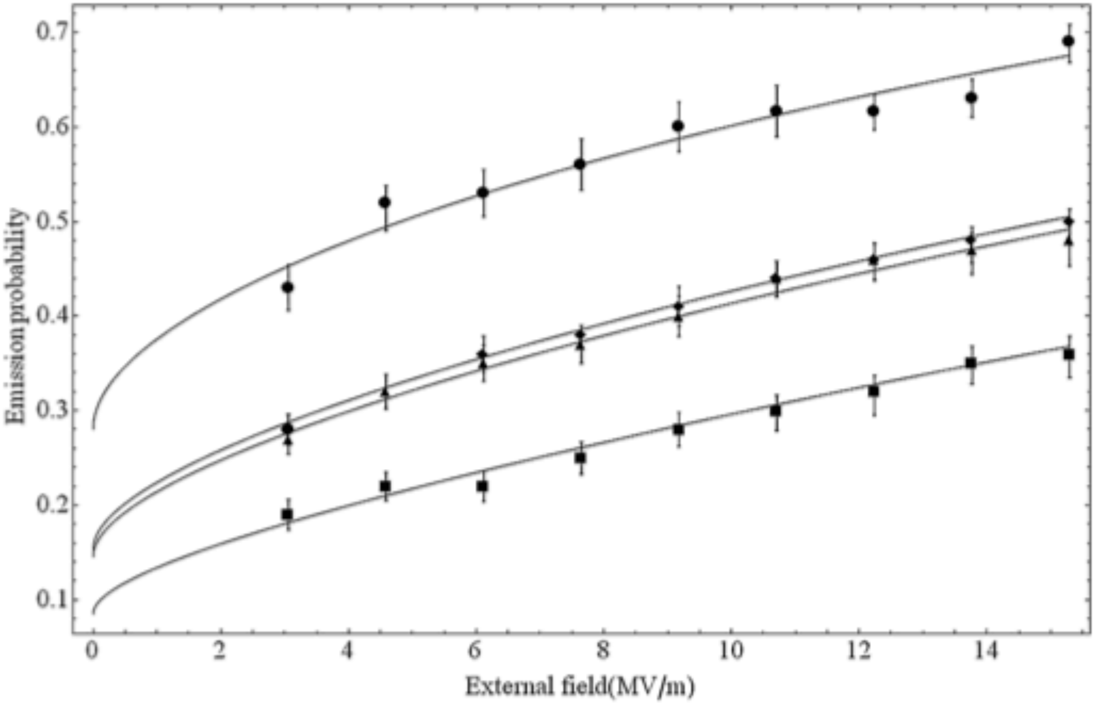
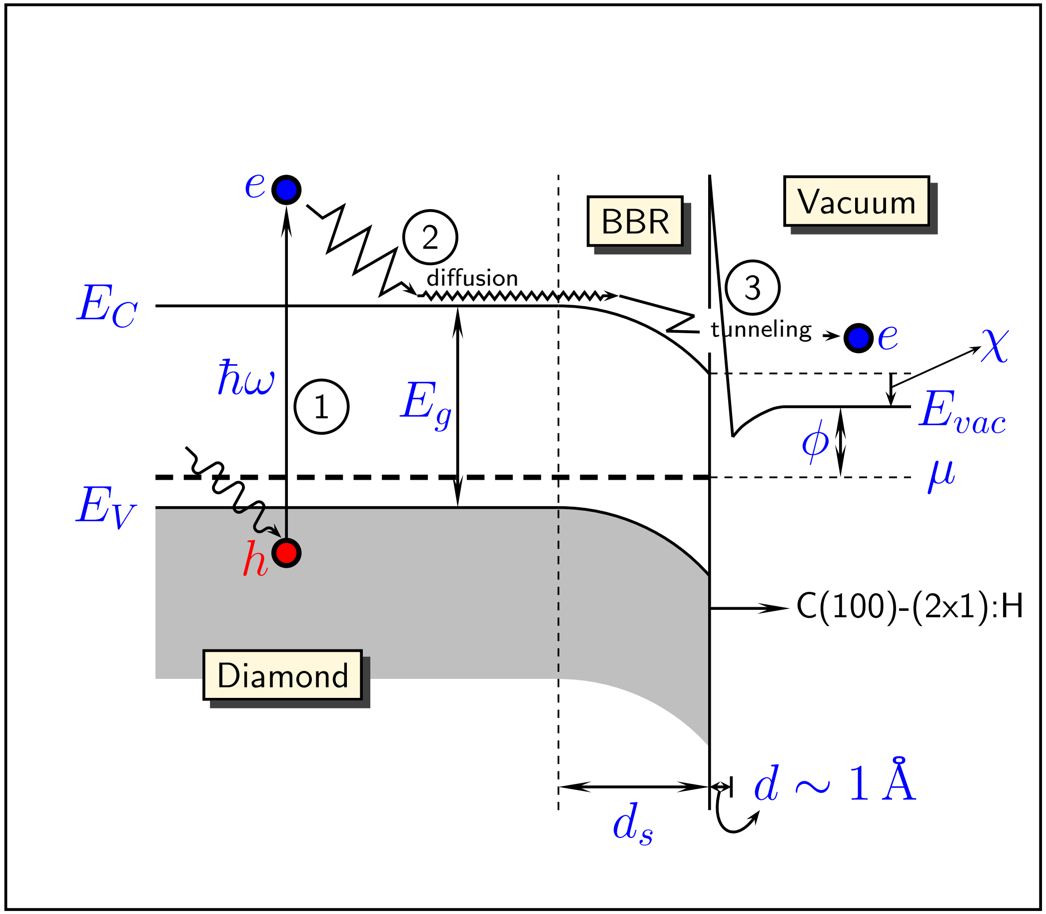


FIG. 3. The dependence of emission probability P on the external field when the pulse width is 200 ns. The points were measured from four different diamond samples. The four solid lines were generated by fitting to Eq. (11), below.

The simulations consist of modeling three main parts.

1. Generation of secondary electrons and holes.
2. Charge transport in a drift-diffusion state.
3. Electron emission from diamond surfaces with varying electron affinity.

- The diagram indicates some of the processes and quantities that the models depend on.



Our approach to model (1) & (2) is described in: D. A. Dimitrov *et al.*, J. Appl. Phys. **108**, 073712-1/12 (2010).

Understanding diamond electron sources requires realistic modeling of emission.

- Initially, we implemented emission from diamond based on a stair-step potential:

$$V(x) = \begin{cases} \chi, x > 0 \\ 0, x \le 0 \end{cases}$$

- Advantages of this model:
  - Analytically solvable quantum mechanically
  - Relatively straightforward to implement
- Disadvantages:
  - Does not include the effect of applied field on surface potential and, thus on the probability of emission.
  - Experimental results from [#] BNL have demonstrated a marked dependence of the probability of emission on applied field.
- Some important limitations of the initial implementation:
  - Did not include the effect of full crystalline momentum in the emission algorithm.
  - Cannot model emission through tunneling (from choice of potential).

We recently implemented more realistic emission models in VORPAL.

- We implemented two new emission models:
  - (/\) - using a triangular potential barrier at the surface (F is the external field and χ is the electron affinity):

$$V(x) = \chi - Fx$$

  - (∩) - and a potential barrier with the image charge effect included:

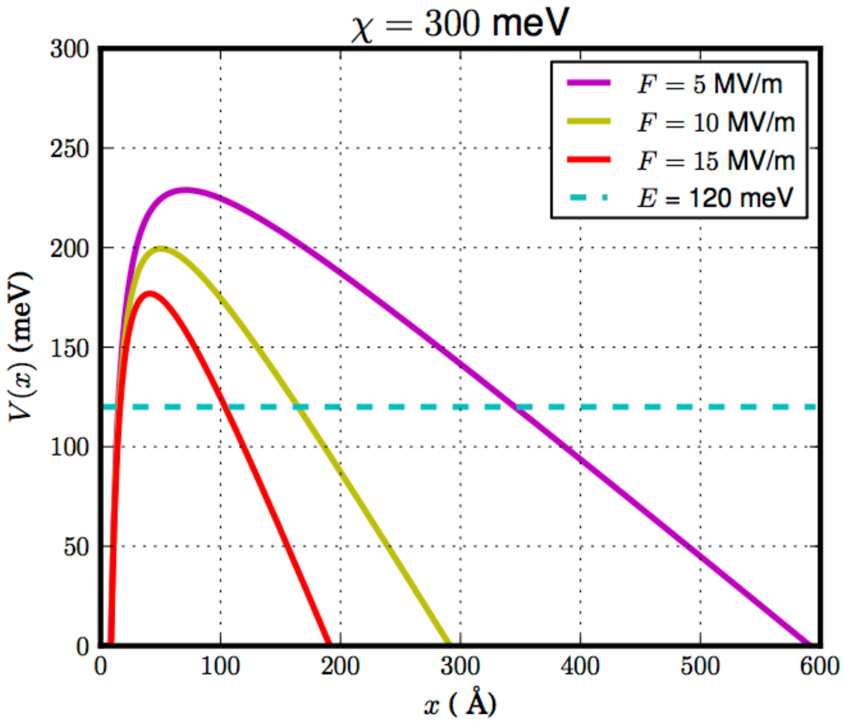
$$V(x) = \chi - Fx - \frac{Q}{x}, \quad Q = \frac{q^2}{16\pi\varepsilon_0} \times \frac{(K_s - 1)}{(K_s + 1)}$$

  - The implementation is based on models developed by K. Jensen *(see, e.g., K. Jensen, J. Vac. Sci. Technol. B,* ***21****:1528–44, (2003); J. Appl. Phys.,* ***102*** *024911, (2007)).*

The new emission models included effects due to the external field.

- For the triangular potential barrier model, (Λ), increasing the magnitude of the external field F, changes the slope of the potential leading to reduction of the tunneling distance during emission (for incident electron energy E < χ).

- Including the image charge to the potential in model (∩), leads to reduction of the potential maximum when increasing the field (shown for three different fields and χ = 300 meV).
- This increases over the barrier emission.



The models calculate the probability for both tunneling and over-the-barrier emission.

- The emission is calculated using an effectively one-dimensional model (we use the energy normal to the emission surface).
- (∧) - triangular barrier:

$$P\left(E\right)=\frac{4\sqrt{E\left|E-\chi\right|_{+}}}{\left\{2\sqrt{E\left|E-\chi\right|_{+}}+\left(E+\left|E-\chi\right|_{+}\right)\left[e^{\theta(E)}-\frac{1}{4}\left(1-e^{-\theta(E)}\right)\right]\right\}}, \qquad (3)$$

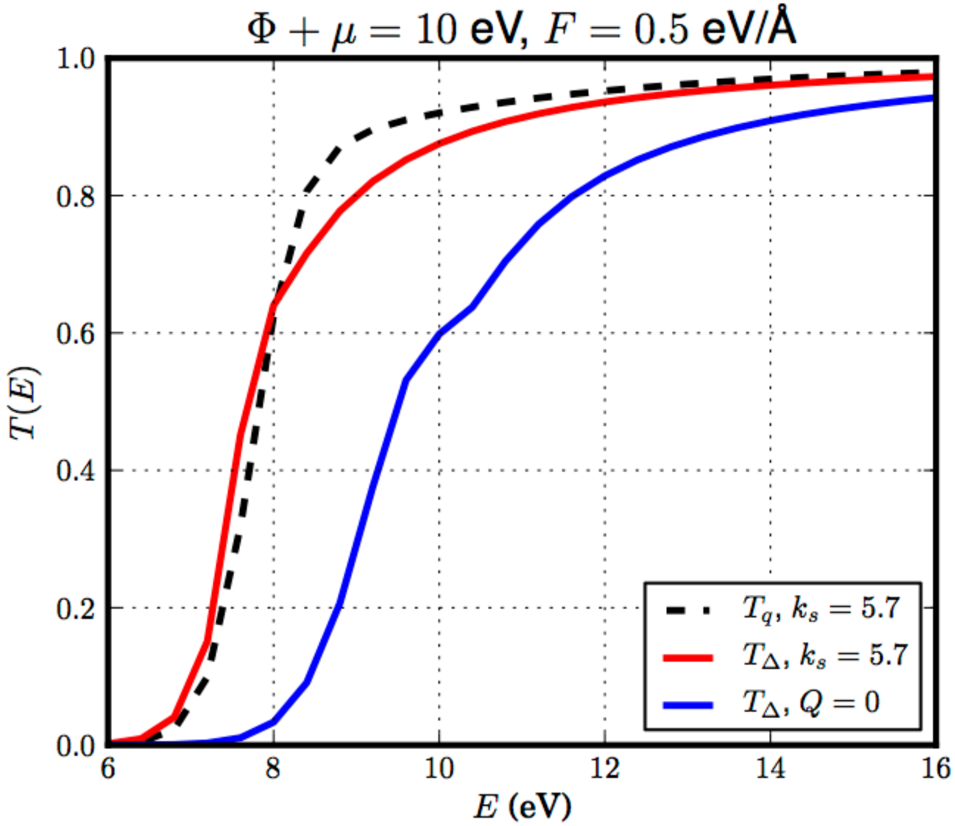
where $\theta(E)=2\sqrt{2m\left(\chi-E\right)^{3}}$ for $E<\chi$ and $\theta(E)=0$ for $E>\chi$, $\left|E-\chi\right|_{+}=\sqrt{\left(E-\chi\right)^{2}+\gamma_{F}}$, $\gamma_{F}=\left(p_0^2\hbar^2F^2/2m\right)^{2/3}$, and $p_0=0.51697$. Note that in the limit of zero field $F\rightarrow 0$, Eq. (3) recovers the emission probability in the stair-step potential.

- (∩) - image charge modifications (*K. Jensen, J. Vac. Sci. Technol. B, **21**:1528–44, (2003)*):

$$T_q\left(E\right)=\frac{C_q\left(E,\chi\right)}{1+\exp\left(2\theta_q\left(E,\chi\right)\right)}$$

The implementation in VORPAL was verified against a previous implementation.

- We verified the implementation for the probability of emission against data from an implementation written previously by Kevin Jensen.



- The transmission probability equation for the triangular potential barrier can be modified to include image charge corrections.
- *K. Jensen, J. Vac. Sci. Technol. B,* ***21****:1528–44, (2003):* "… for $K_s > 2$, $T_q(E)$ is superior, but for $K_s \approx 1$, $T_\Delta(E)$ is superior."

The emission/reflection algorithm proceeds in three main steps.

① Check if the particle push solver attempts to move a particle across the emission surface.

② If yes, calculate the probability of emitting the particle

③ Attempt the emission of this particle with the calculated probability using a Monte Carlo approach

④ If proceeding with emission, emit the particle only if:

  i. Transverse momentum (in the emission plane) can be conserved

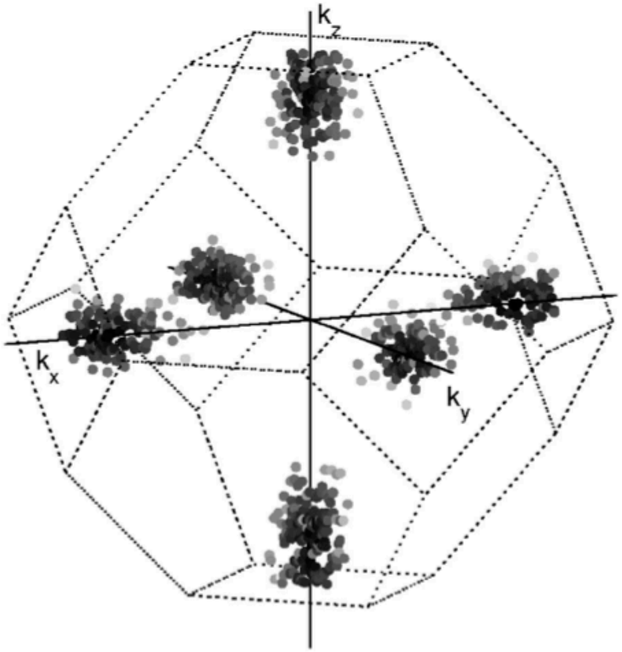
  ii. Energy can be conserved (tunneling and over the barrier emission are handled separately)

⑤ Otherwise, reflect the particle at the emission surface and move it to its final position (in diamond)

Emission is significantly affected by conservation of transverse momentum.

- Emission from a (100) diamond surface is practically allowed only from two of the six equivalent conduction band energy valleys.
- The conduction band minimum is at $k_{\alpha 0} \approx 0.73\times(2\pi/a)$ with $a \approx 3.57$ Å.
- An electron not in the two valleys along [100], will have to be emitted with energy of at least about 6.3 eV, $(\hbar k_{\alpha 0})^2/(2m_e)$, to conserve its transverse momentum.
- However, max gain from NEA is < 1.3 eV, and energies in diamond are typically less that several 100 meV since they depend on the momentum relative to the minima:

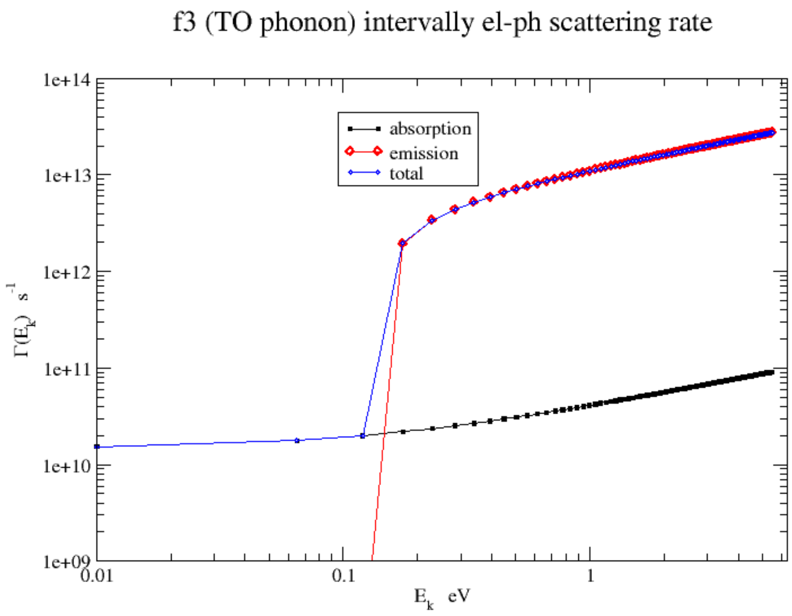
$$E_{010}(k) = \frac{\hbar^2}{2m_T}\left(k_x^2 + k_z^2\right) + \frac{\hbar^2}{2m_L}\left(k_y - k_{y0}\right)^2$$



Electron distribution in momentum space from modeling Si (fcc lattice similar to diamond), E. Pop *et al.*, J. Appl. Phys. **96**, 4998 (2004).

Electrons on transverse valleys can scatter to the (100) valleys and then be emitted.

- There are two electron-phonon scattering processes that allow transitions between perpendicular valleys (Jacobony & Reggiani, Rev. Mod. Phys. (1983)) with phonon energies:
    - 0.13 eV (LA, f2 mode) & 0.15 eV (TO, f3 mode)
    - Average time for such transitions (via phonon emission) is ~ 0.1 ps.
- Another phonon-assisted emission mechanism was proposed by J. Rameau *et al.* [##] that we have not considered so far.



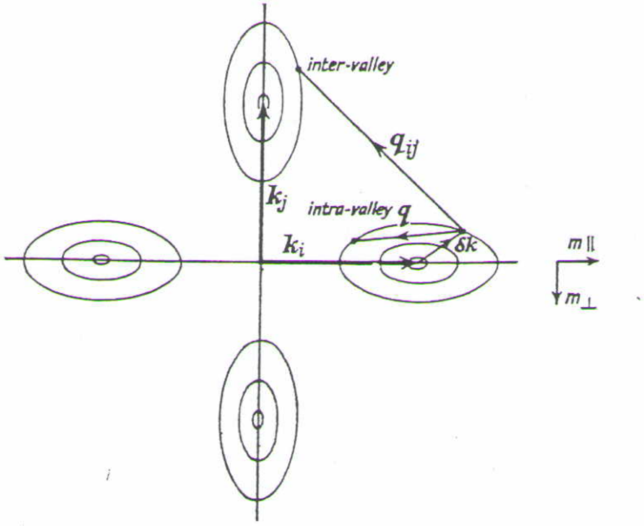
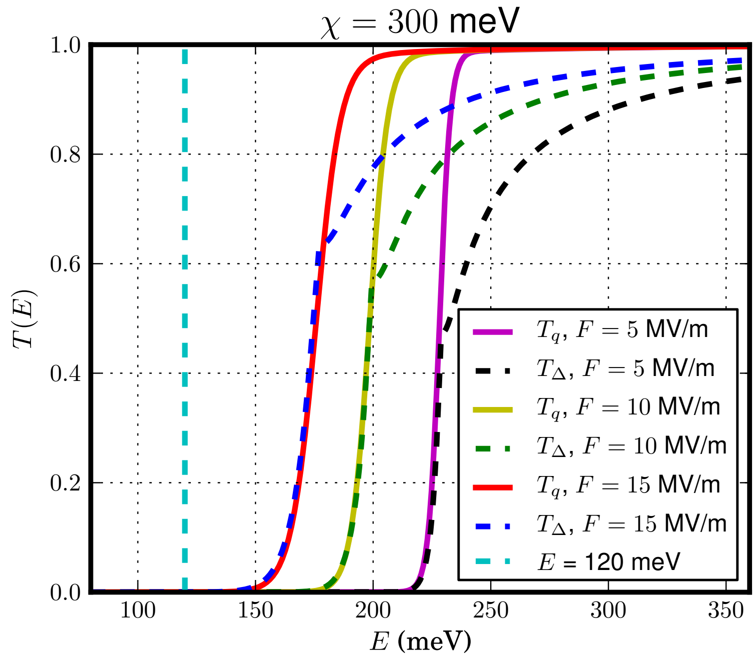


FIG. 137. The many-valley model, and the types of scattering process.

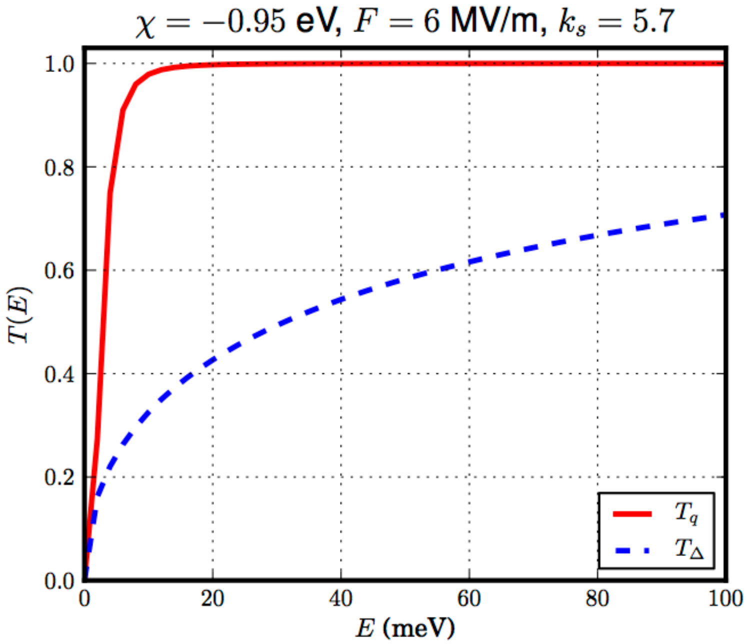
J. M. Ziman, Electrons and Phonons (1962).

The probability of emission depends strongly on the electron affinity and the external field.

- Emission probabilities calculated with the new emission models indicate the electron energies needed for emission at different applied fields:
  - The onset of emission for “effective NEA” shifts markedly when changing the external field.
  - For “true NEA”, only conservation of transverse momentum limits emission.



“Effective NEA”



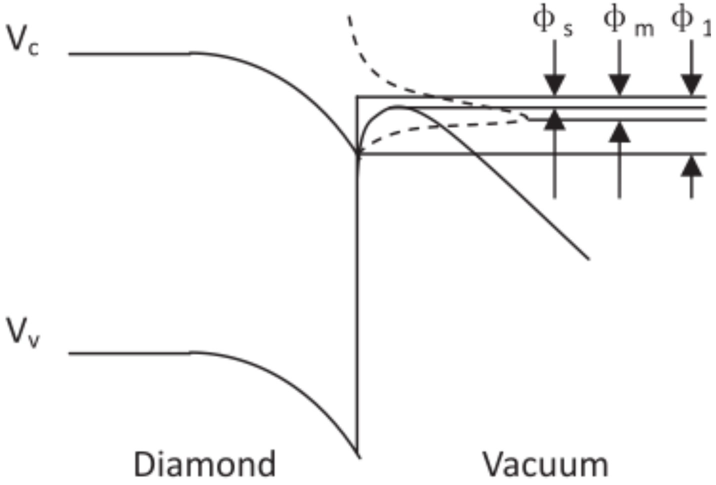
“True NEA”

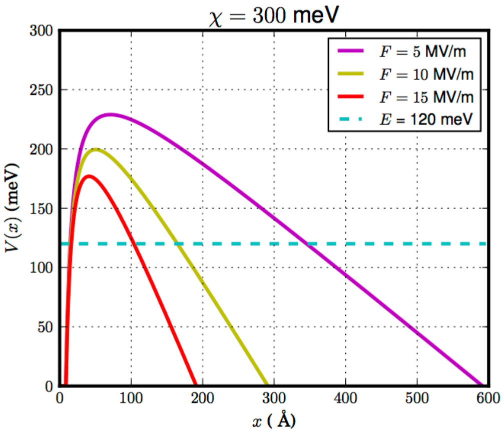
The proposed interpretation of emission data considered "effective NEA".

- "Effective negative electron affinity" is defined by a vacuum level lower than the conduction band minimum (CBM) in bulk diamond but higher than the CBM at the emission surface.
- This is possible due to downward band bending at the surface.

Downward band bending W ≈ 0.4 eV was measured at a (100) hydrogenated surface of boron-doped diamond (F. Maier *et al*., Phys. Rev. B **64**, 165411 (2001)).

$$f(\varphi) = \frac{e^{-[(\varphi - m)^2/2\sigma^2]}}{\sqrt{2\pi\sigma^2}},$$

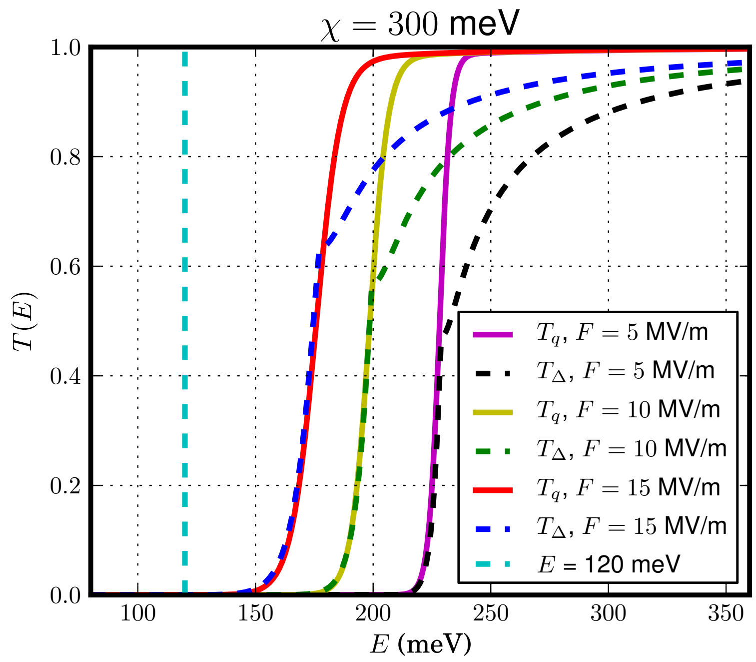


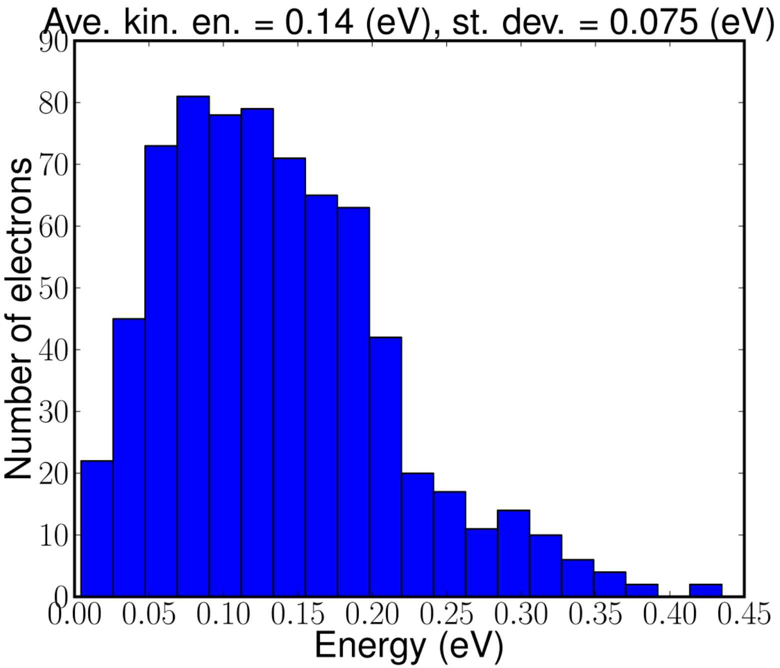


Given the new emission modeling capabilities (and within the current overall simulation limitations), we wanted to model this system to understand how it compares with measured experimental data.

Simulations in bulk diamond indicate the fraction of electrons that could be emitted.

- The probability of emission as a function of energy and external field calculated with the implemented models show the minimum electron energy when emission is realistically possible.
- Electron energy distributions from transport simulations in bulk diamond provide information about the fraction of electrons that could be emitted (sample distribution is from simulations with 1.8 MV/m field in diamond).





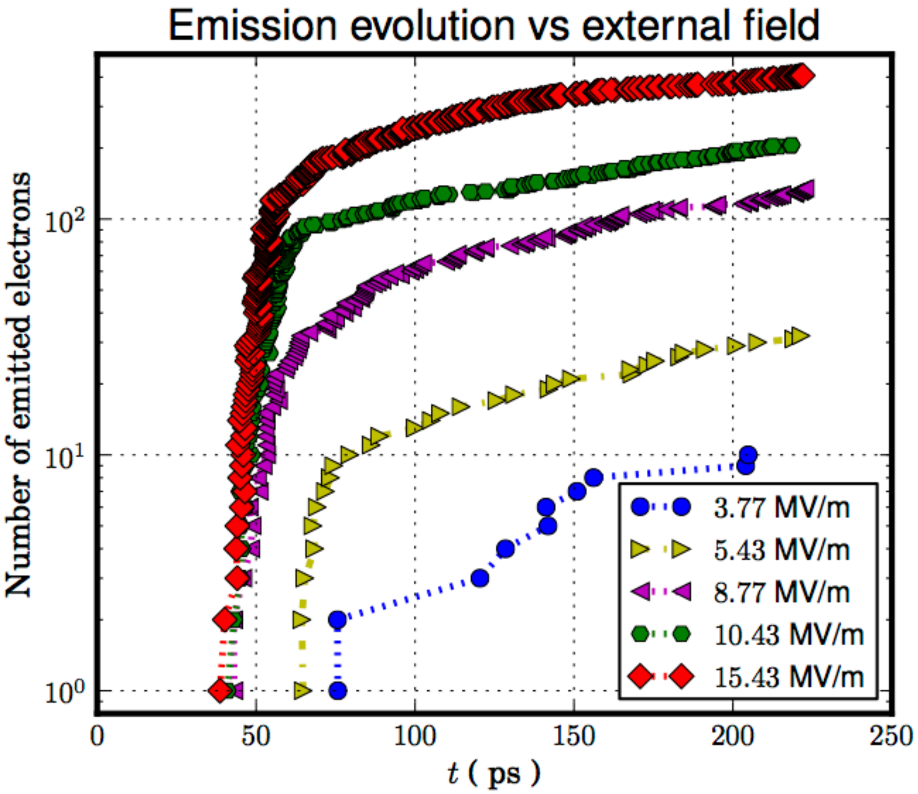
VORPAL simulations were done with and without band bending.

- Selection of some essential simulation parameters:
  - The external field was varied in the range from 2.1 to 17.1 MV/m
  - Most of the current simulations were with electron affinity of 0.3 eV.
  - A single primary electron with energy E_p = 9 keV was used to generate the secondary electrons
  - $N_{tr} \approx 600$ total electrons are eventually transmitted to the emission surface of the diamond slab.
  - Without band bending: 8×12×12 μm, 40×30×30 cells along x, y, z; diamond length (along x): 6.5 μm, vacuum length: 1.5 μm.
  - With band bending: 4×12×12 μm, 161×30×30 cells along x, y, z; diamond length (along x) ≈ 3.091 μm, vacuum length ≈ 0.090 μm, band bending region with W = 0.36 eV and length d = 0.1 μm.

Emission slows down after the initial energetic electrons in the (100) valleys are emitted.

The emission probability was estimated from $P = N_{em}/N_{tr}$, where the number of emitted electrons was collected over a time interval of about 170 ps.

Electrons from the perpendicular valleys can transition to the (100) valleys due to electron-phonon scattering (average time for such a transitions via phonon emission is ~ 0.1 ps) and could be emitted.

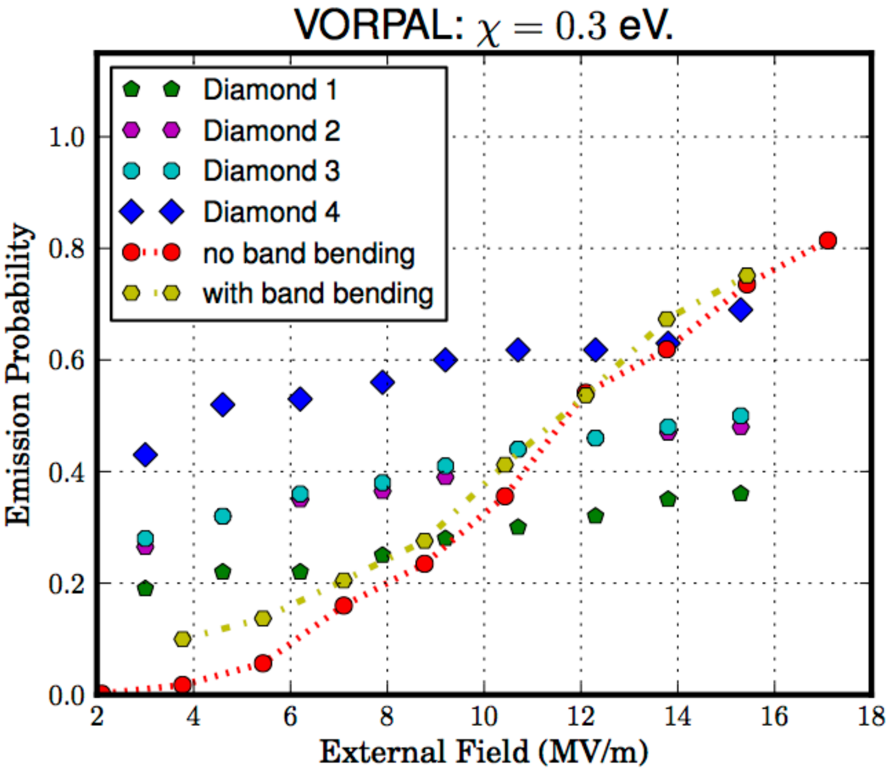


The current simulations have some important limitations.

- Surface roughness effects are known to be important but we have not implemented models to include them.
- The simulations are over a relatively short period of time and do not take into account the transport of secondary electrons when the field in diamond decreases due to accumulation of charge at the emission surface.
- Metal contacts are not modeled.
- Modeling of emission from localized states that arise in the band bending region near the emission surface is not included.
- Modeling of direct phonon-assisted emission, as suggested by J. Rameau *et al.* (2011) is not included.

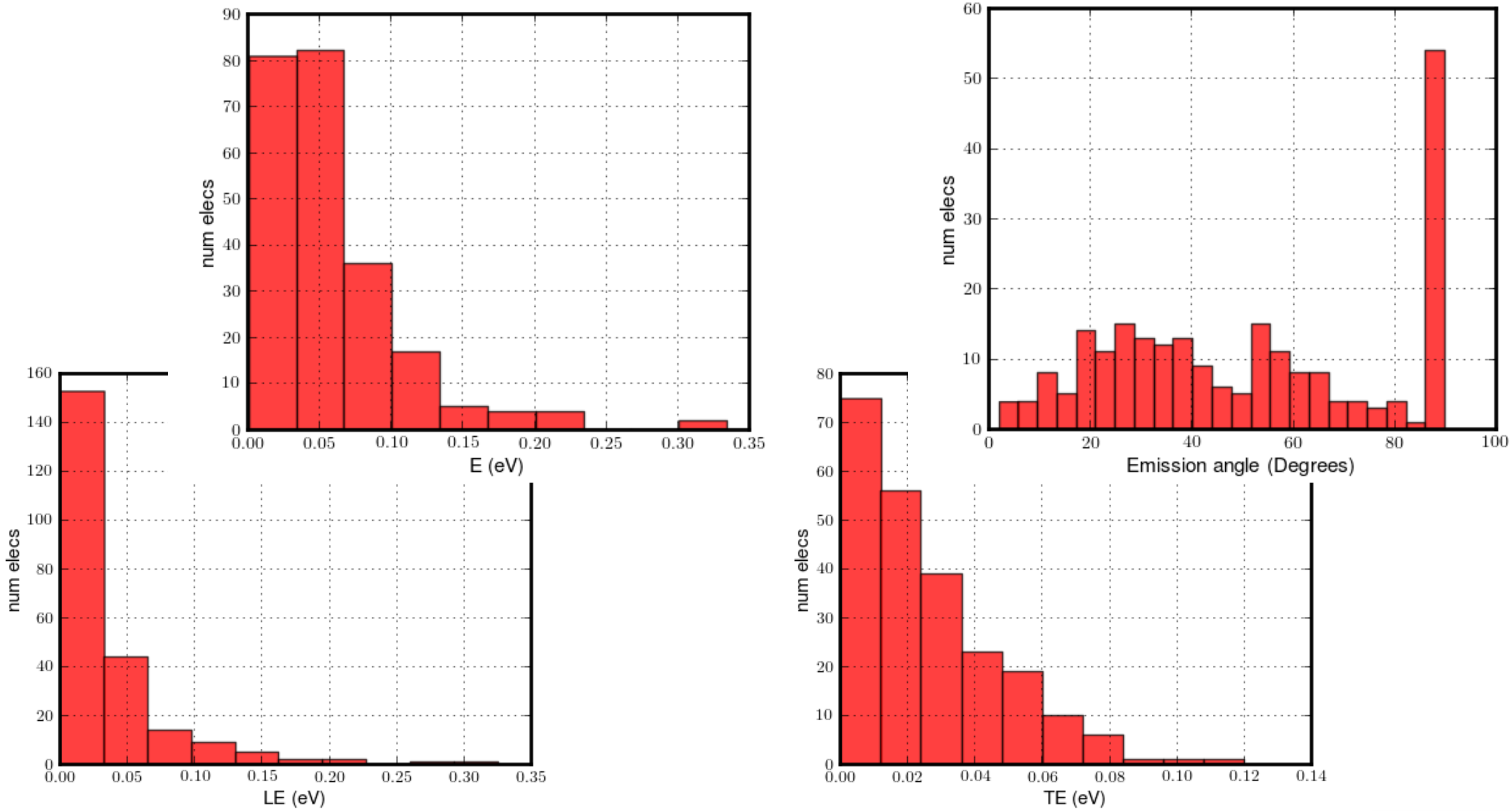
Results from the VORPAL simulations are in qualitative agreement with the experimental data.

- Even without a number of important effects not included in the models, the simulation results show qualitative agreement with the experimental data from BNL.
- The electron affinity and external field are the main parameters given as input to the models.
- Given the variation in the probability of emission from different diamond samples, we expect that including modeling of surface roughness effects and surface-varying electron affinity (as previously suggested by J. B. Cui *et al.*, Phys. Rev. B **60**, 16135 (1999)) will lead to improved agreement with the experiments.



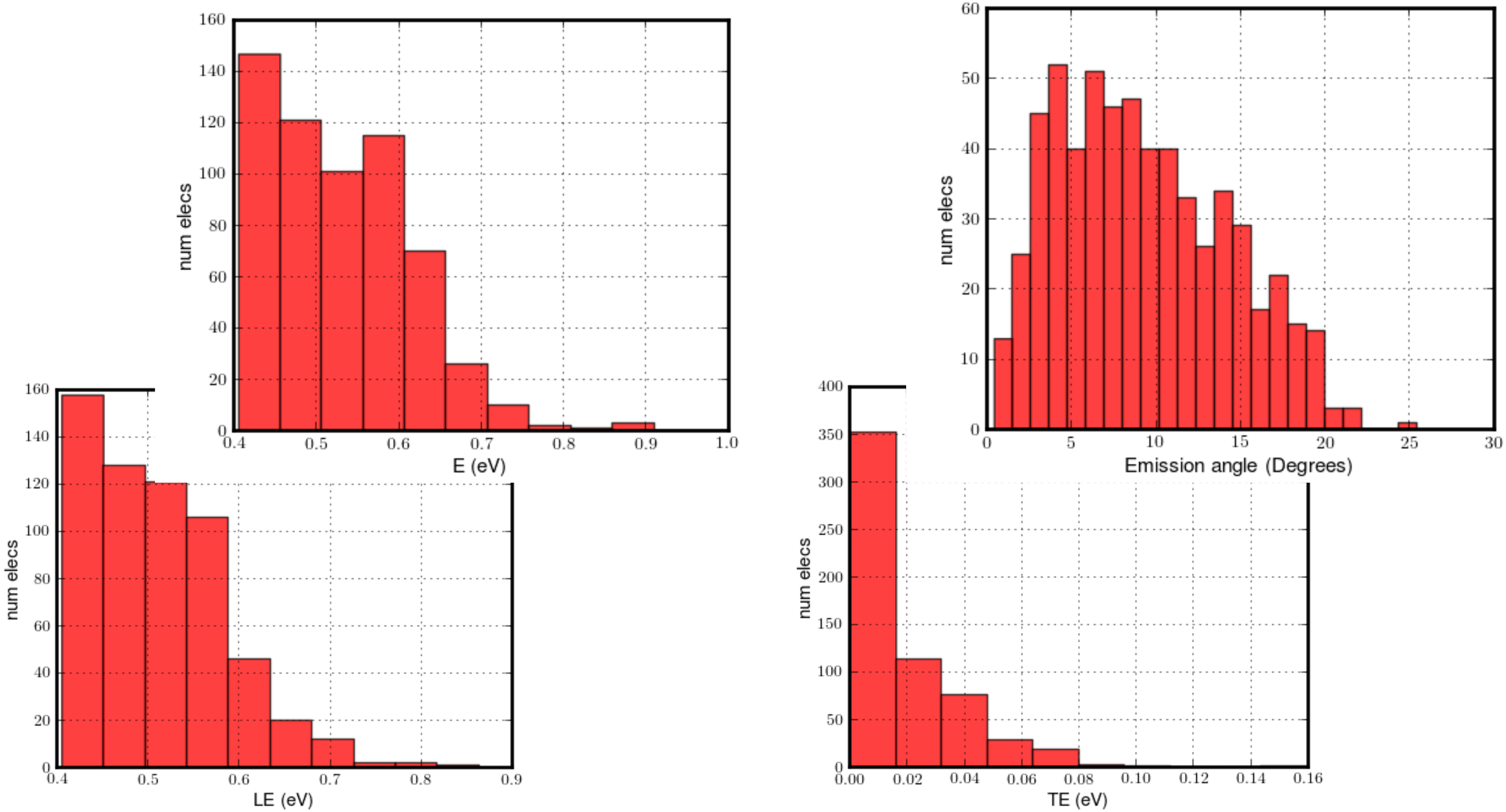
Tunneling affects the energy distribution of emitted electrons (data for χ = 0.3 eV).

The peak at $\pi/2$ in the angular distribution is due to emission via tunneling.



The angular distribution is narrower for emission from a true NEA surface (data for χ = -0.3 eV).

The energy spread, as expected, is broader.

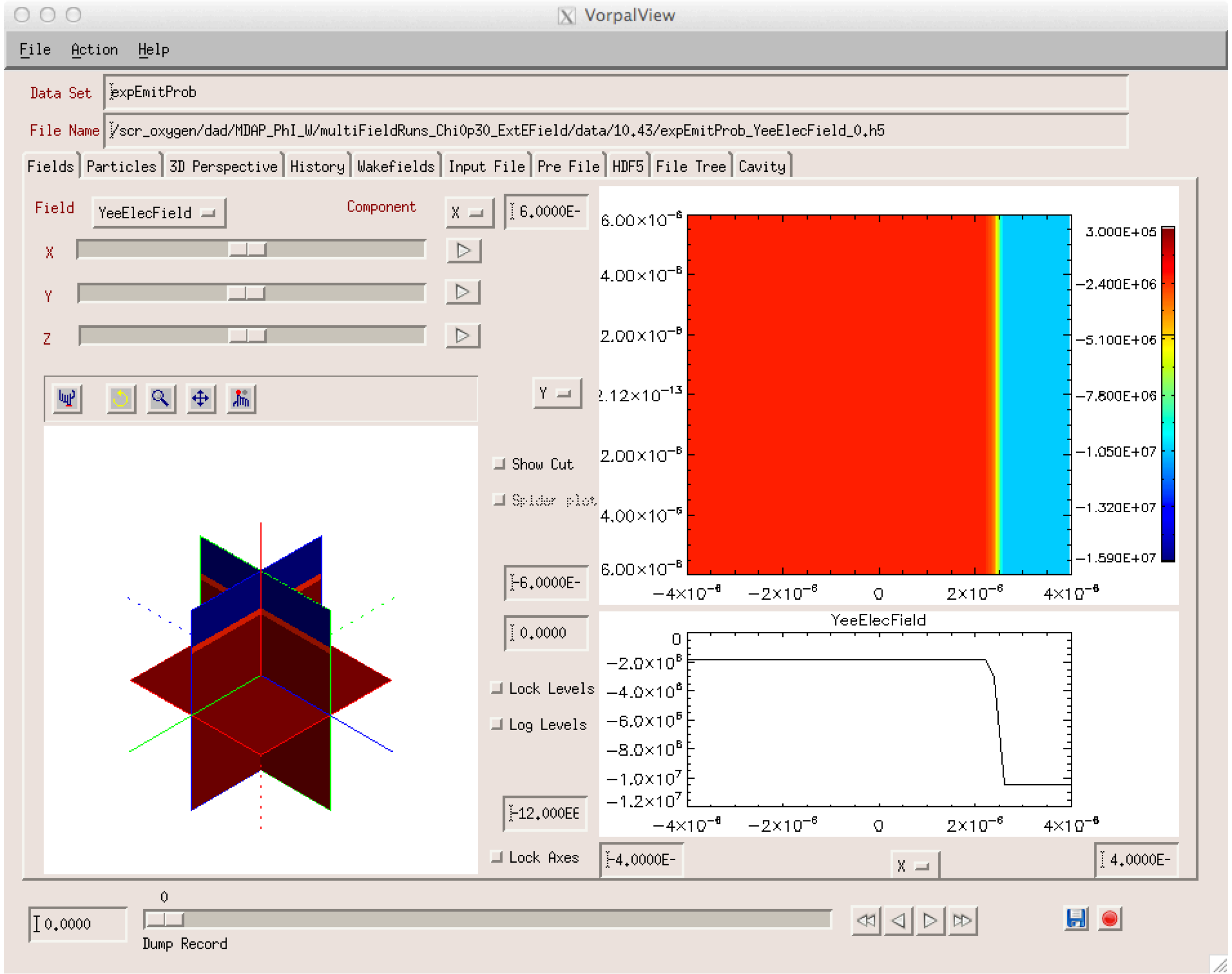


Summary and Future Work

- We have implemented more accurate models for emission of electrons from diamond
- The emission probability depends on the external field and includes image charge corrections.
- The probability of emission obtained from the simulations is in qualitative agreement with the experimental data.
- This indicates that the observed behavior of electron trapping near the emission surface could be due to effective negative electron affinity close to 0.3 eV.
- It is essential to include in the modeling the six equivalent conduction band valleys, their effective masses, and conservation of transverse momentum during emission.
- The current modeling has important limitations - we expect that including surface roughness effects and surface-varying electron affinity will improve the agreement with the experimental data.

A primary electrons enters from the left side in a given initial field distribution.

The diamond slab is 6.5 μm long and the vacuum region is 1.5 μm.



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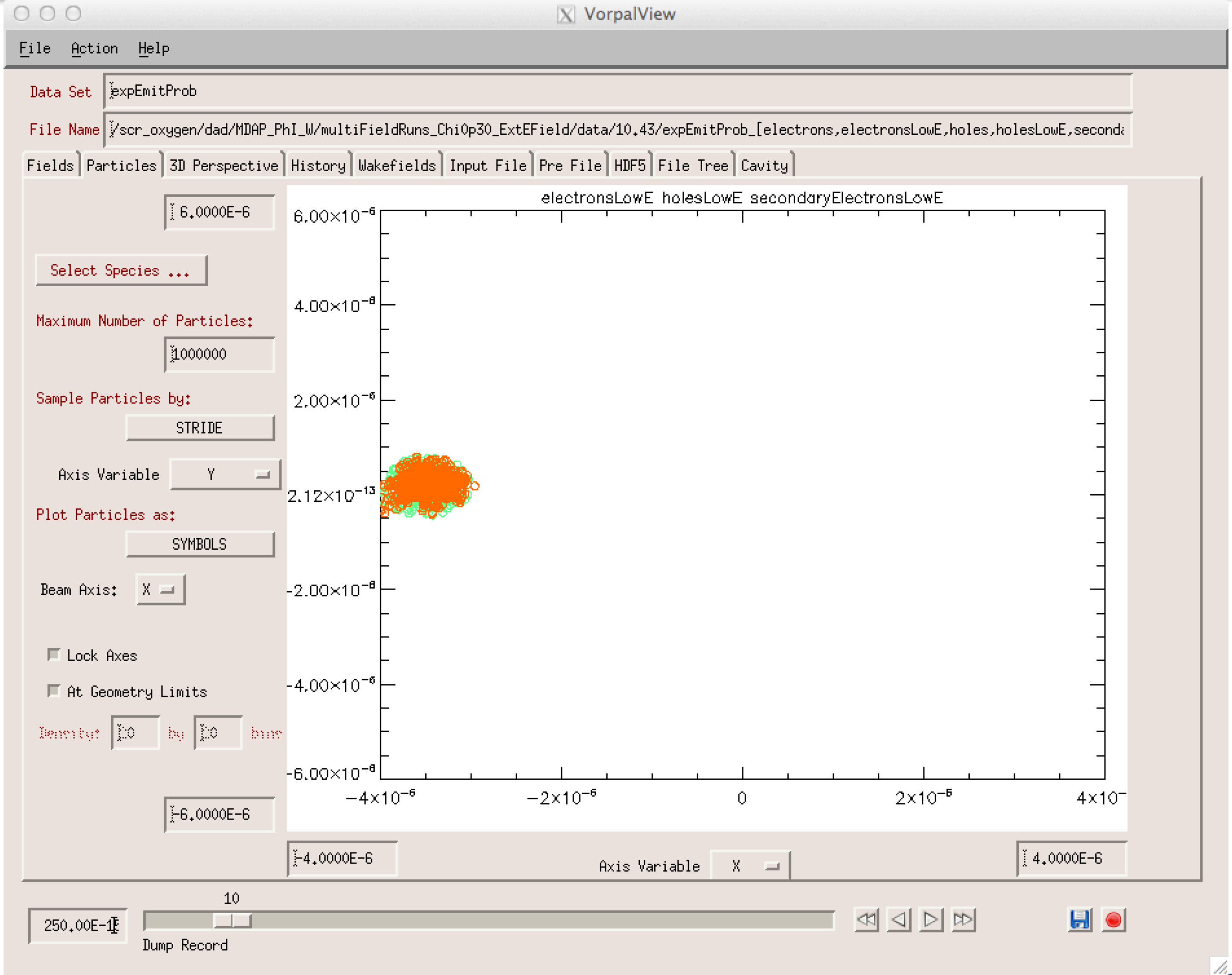
Field: YeeElecField

Component: X

Secondary electron and hole generation phase completes in about 250 ps.



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6.0000E-6

Maximum Number of Particles: 1000000

Sample Particles by: STRIDE

Axis Variable: Y

Plot Particles as: SYMBOLS

Beam Axis: X

-6.0000E-6

-4.0000E-6

Axis Variable: X

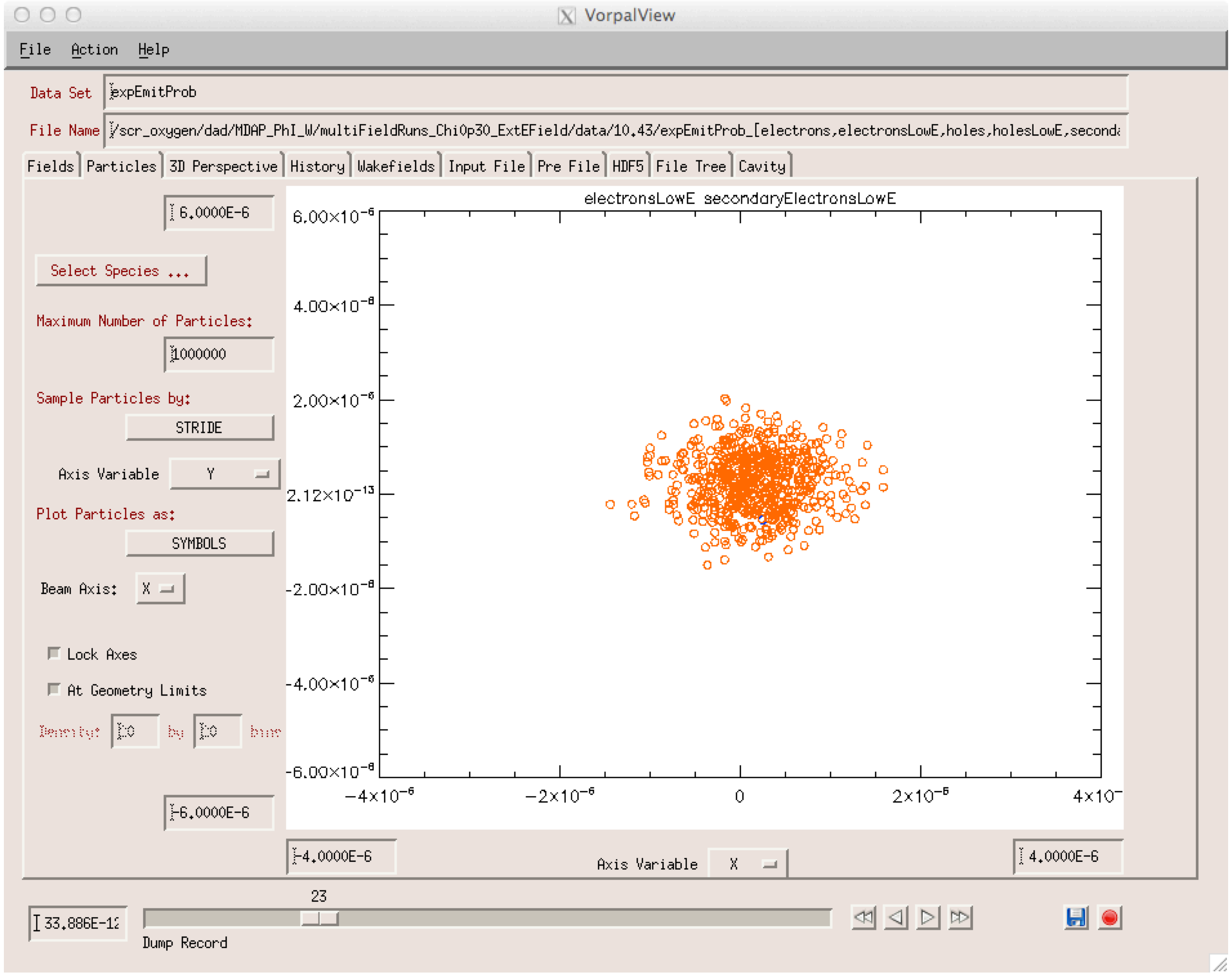
4.0000E-6

250.00E-12

Dump Record: 10

Electrons settle in a drift state moving towards the emission surface.

The number of transmitted electrons is determined from counting their number in the drift state.



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Maximum Number of Particles: 1000000

Sample Particles by: STRIDE

Axis Variable: Y

Plot Particles as: SYMBOLS

Beam Axis: X

☐ Lock Axes

☐ At Geometry Limits

Axis Variable: X

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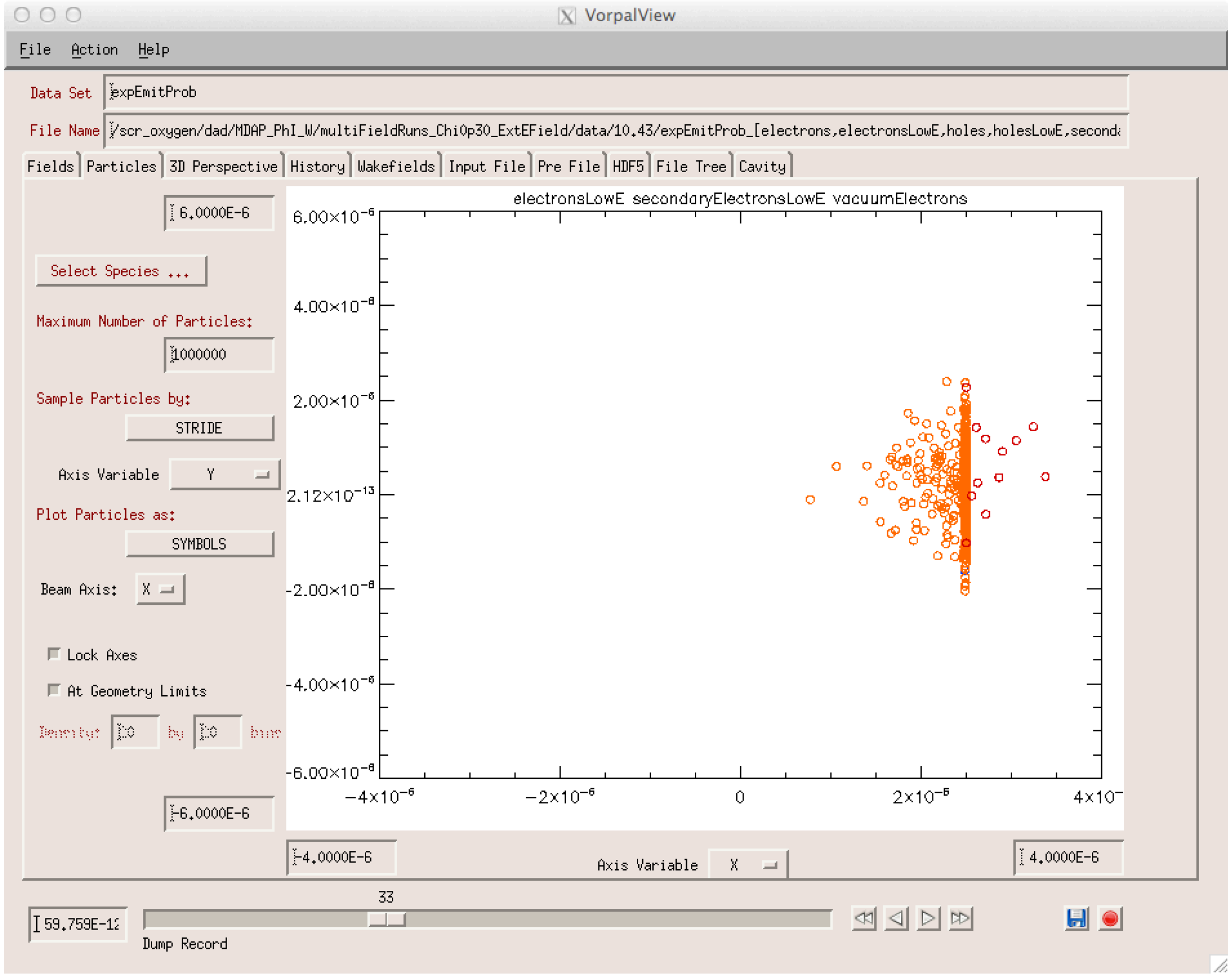
Early emission reduces the energetic electrons in the 100 valleys.

Other electrons are reflected and accumulate near the emission surface.



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electronsLowE secondaryElectronsLowE vacuumElectrons

6.0000E-6

Maximum Number of Particles: 1000000

Sample Particles by: STRIDE

Axis Variable: Y

Plot Particles as: SYMBOLS

Beam Axis: X

☐ Lock Axes

☐ At Geometry Limits

Density: 0 by 0 bins

-6.0000E-6

-4.0000E-6 Axis Variable: X 4.0000E-6

59.759E-12

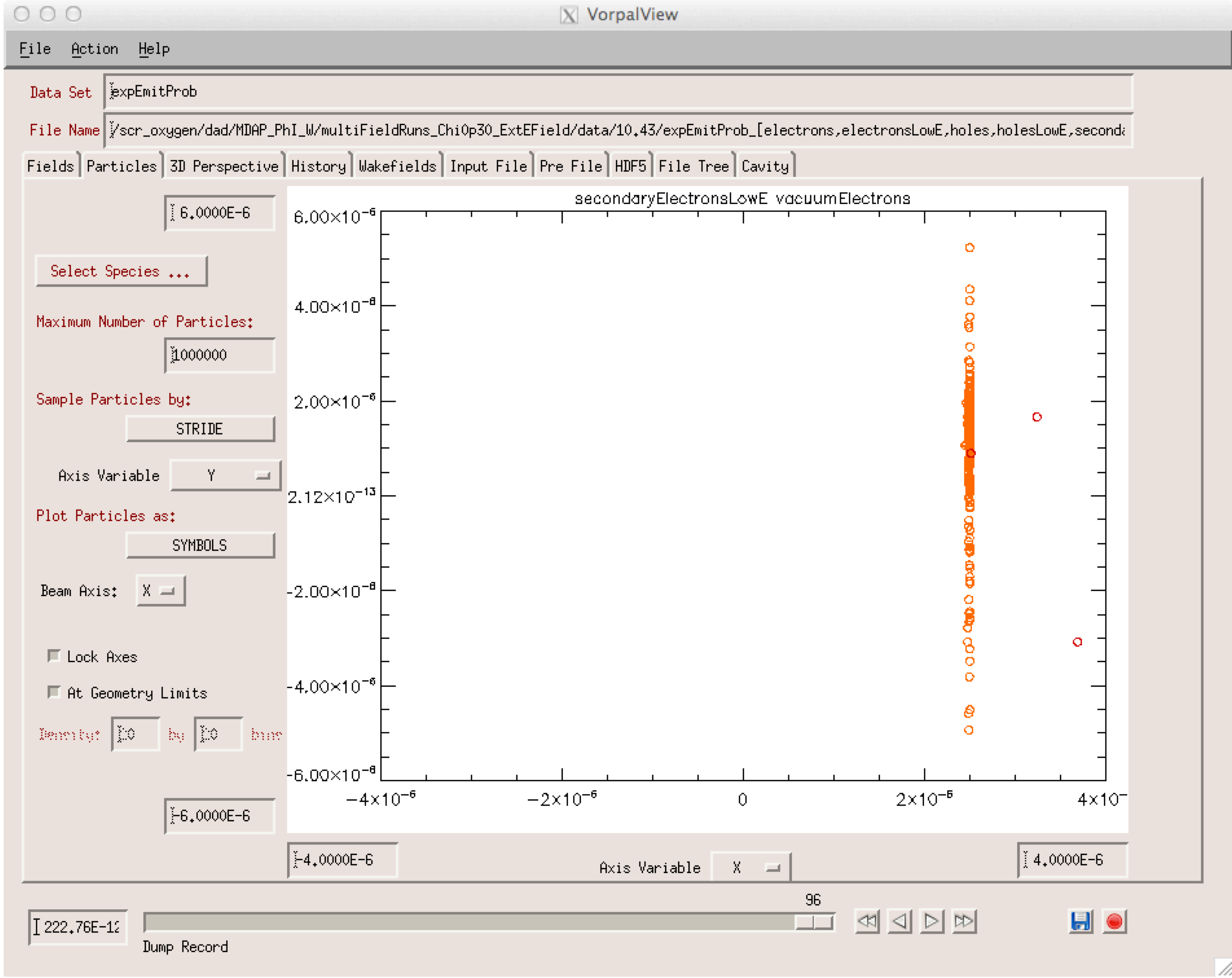
33

Dump Record

Later stage emission is assisted by electron-phonon scattering.

- Electron-phonon transitions between perpendicular valleys allow electrons to get to the 100 valleys that could then be potentially emitted.

- The emission is slowed down in this regime and the conduction band electrons in diamond are effectively trapped near the surface.



VorpalView

Data Set: expEmitProb

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Maximum Number of Particles: 1000000

Sample Particles by: STRIDE

Axis Variable: Y

Plot Particles as: SYMBOLS

Beam Axis: X

☐ Lock Axes

☐ At Geometry Limits

Density: 0 by 0 bins

Vertical limits: 6.0000E-6, -6.0000E-6

Horizontal limits: -4.0000E-6, 4.0000E-6

Axis Variable: X

222.76E-12

Dump Record: 96