Emission models and beam dynamics for diamond emitters in a compact source of high brightness beams


Los Alamos National Laboratory

2018 Photocathode Physics for Photoinjectors (P3) Conference
Santa Fe, NM, USA
10/17/2018
Diamond field emitter as an enabling technology for Dielectric Laser Accelerator

**Breakdown limits**

- **PWFA/LWFA**
- **CW Laser**
- **Infrared laser** e.g., $\lambda \sim 1-10\mu m$
- **Woodpile structure**
- **Diamond field emitter cathode**
  - e.g., 10ps UV (4eV, 0.4mJ/pulse)

Adapted from B. Hidding et al., Phys. Plasmas 16, 043105 (2009)
Structure and emission characteristic of diamond field emitter

- Understanding of the emission regimes (i.e., field and photo emission) in micron- to nano-scale structured materials. **Challenges**: material, topology, transport

- Beam dynamics in field or photo emission from the pyramid and the nano-tip

- Scalability of emission properties for assemblies of emitters
Overview of the integrated diamond emitter simulation model

- Photo excitation
- Nano-tip
- Bulk Material
- Diamond pyramid photo-cathode
- Emission model for nano-tip
  - Conduction Band
  - Vacuum
  - Valence Band
  - Tip Quantum Confined Electronic Structure
  - Auger-Assisted Ionization Process
- Emission model for the bulk
  - Conduction Band
  - Valence Band
  - Bulk band Structure
  - Bulk-Vacuum Interface emission

Finite element ES solver and FDTD EM beam transport simulation (LSP)

Child-Langmuir, Fowler-Nordheim, Murphy-Good
Beam current, energy spread and dynamics from self-consistent electromagnetic simulation with the Murphy-Good emission law

**Electric field**

Vector Plot of $E$ at $T_n = 6.283; t = 0.1091$

Diode voltage = 0.4 kV
AK gap = 33 μm
$E = 120$ kV/cm

**Electric potential**

Potential integrated from $E_z$ at $T_n = 6.283; t = 0.1091$

**Emitted current**

Emission model: Murphy-Good (FN + thermionic emission)

$I = 30 \mu$A

**Emitted beam**

Outside layer has most beam current

**Kinetic Energy vs Z**

At the anode:
$\Delta E = 25$ eV
$\Delta E/E = 6.6\%$

**Transverse velocity vs Z**

Operated by Los Alamos National Security, LLC for NNSA
3-D LSP simulation of single tip pyramid with different emission areas

Emission is allowed over the first two cells in the emitter

Emission is allowed over the first cell in the emitter

Beam current (mA) - MG

Beam Current (mA) - CL

LSP simulations indicate that only a small area at the tip of DFE responsible for electron emission

~1.3mA/emitter @114kV/cm

~15.6mA/emitter @114kV/cm
Emission properties of nanodiamond flat film depend on deposition process

(a) 550°C
(b) 600°C
(c) 650°C
(d) 700°C
(e) 750°C
(f) 800°C

Nanodiamond Field Emitter Arrays exhibit similar emission properties

1.1e6 tips array, RF gun
4um base, 10um pitch
15mA at 30MV/m (0.014 uA/tip)
1e-9 Torr
Unconditioned

7x7 array, DC
3um base, 10um pitch
0.1mA (2uA/tip) at 10MV/m
1e-6 Torr
Unconditioned

5x5 array, DC
10um base, 100um pitch
5.5uA/tip at 11MV/m
15uA/tip at 15MV/m
1e-9 Torr
High current (>1 uA/tip) conditioned

20MV/m 10MV/m

1.5e5 tips array, DC
12um base, 10um pitch
22mA at 10MV/m (0.15 uA/tip)
1e-6 Torr
Unconditioned


Electron transport in diamond modeled with Monte-Carlo method

- Scattering processes in the Monte-Carlo transport
  - Three-valley model for diamond electronic structure
  - Phonon scattering (intravalley scattering with acoustic and nonpolar/polar optical phonons and intervalley (with acoustic and optical phonons),
  - carrier & impurity scattering can be included

- Simulated electron mobility is validated for diamond
Emission from surface tunneling modeled with the Transfer-Matrix approach

- Energy/momentum conservation and anisotropic effective mass effect included in the Transfer Matrix method for electron tunneling

\[ E_{(010)}(k) = \frac{\hbar^2}{2m_T} (k_x^2 + k_z^2) + \frac{\hbar^2}{2m_L} (k_y - k_0)^2, \]

\[ E_{\text{vac}} = \left( \frac{\hbar k_0}{2m_e} \right)^2 \approx 6.3 \text{ eV}, \]

Semiconducting emission characteristics from Monte-Carlo + tunneling simulations applied to micron-scale emitter: preliminary result

Field enhancement factor vs tip aspect ratio

Current density across the pyramid & tip surface

\[ \beta = \beta_{\text{pyramid}} \beta_s \]

\[ \beta_s = 1 \quad \beta_s = 5 \]

Bulk diamond emission characteristic

\[ I = 11.35 \exp(0.0114 \times E [\text{MV/m}]) \]

Fraction of total current vs. fraction of emitting area

\[ \frac{h}{h_0} \]
Nano-tip transport model

- Approximate tip as a set of Nano-wires (NWs) of different radii:

  
  
  
  
  

- Set of 1D Boltzmann equations for NW:

  

  \[
  \frac{\partial f_{n\alpha}(z, k_z)}{\partial t} + \frac{\hbar k}{m^*_L} \frac{\partial f_{n\alpha}(z, k_z)}{\partial k} + \frac{\partial k}{\partial t} \frac{\partial f_{n\alpha}(z, k_z)}{\partial k} = \left[ \frac{\partial f_{n\alpha}(z, k_z)}{\partial t} \right]_c
  \]

  - inter-subband scattering changes momentum $k_z$.

- Account for the NW junction effects via collision integral

  
  
  
  

  back scattering rate

  forward scattering rate

  Scattering probability (L→R)

  \[
  E_{n\alpha}(k_z) = \frac{\hbar^2 \kappa_{n\alpha}^2}{2m^*_T} + \frac{\hbar^2 k_z^2}{2m^*_L}
  \]
Phonon scattering rates calculated for:
- segment radii: L: 6nm; R: 4nm
- scattering segment length: 1nm

Nano-tip transport: preliminary result

Physics-based emission model in RF gun simulation

Goal: high-fidelity *end-to-end* (photo excitation to beam forming) modeling tool validated with published results and experiment observations.

SLAC ACE3P is chosen due to its demonstrated multi-physics and geometric modeling capabilities and high accuracy.

Potential applications:
- physics issues (e.g. emittance degradation, lifetime and emission delay) in semiconductor cathode guns
- validation against experiments and comparison with simplified/ad-hoc emission models currently used in accelerator design;
- detail design capability for gun performance optimization.
Summary

- **Various factors may play important roles in the emission of a diamond emitter**
  - Accurate determination of field enhancement factor <= high resolution FDTD EM and FEM ES simulation
  - Accurate determination of emission area <= diamond emission characteristic from MC + tunneling model of the transport/emission, combined with high resolution simulation
  - Emission from nano-tip <= A new carrier interface transport/emission model for nano-scale structure
  - Beam dynamics <= self-consistent simulation with known emission laws

- **Implications and next steps**
  - Complete and benchmark model to calculate the electron emission current at nano-tip;
  - Implement optical transitions to excited states & photo-ionization processes. (Photo-emission problem);
  - Combine bulk & nano-tip transport and emission models with MC solution for integrated DFE modeling of experiments
Thank you for your attention and look forward to opportunity to collaborate on emission model validation and photocathode gun study!
Electric fields in LSP simulation, after subtraction of the parallel plate solution, can be described by simple scaling.

\( E_r = 0.025/(r+1e^{-5}) \)

\( E_\theta = 0.025*(2.1*\theta/\pi)/(r+1e^{-5}) \)

This finding can be used to simplify trajectory analysis and divergence scaling (next step) without resorting to detail simulation.
Monte-Carlo semi-classical electron transport model for bulk diamond

Brillouin zone

\[ |k_{a0}| \approx 0.73 \times (2\pi/a) \text{ where } a = 3.57\,\text{Å} \]

In bulk diamond, conduction band electrons populate in valleys and experience intervalley scatterings and acoustic scatterings.

\[ \hbar \frac{d\vec{k}}{dt} = -e(\vec{E} + \vec{v} \times \vec{B}), \]
\[ \vec{v} = \frac{1}{\hbar} \nabla_{\vec{k}} E, \]
\[ \frac{d\vec{r}}{dt} = \vec{v}, \]

Intervalley scattering

Intravalley acoustic scattering
Monte-Carlo semi-classical electron transport model for bulk diamond: simplification & parameters

(1) For high purity diamond, hypothesis is that carrier transport is controlled by lattice scattering only.

(2) The lattice scattering, i.e., acoustic and intervalley phonon scattering are the only ones considered, optical phonon interaction being forbidden by symmetry arguments [8].

(3) The intervalley phononenergies for g-type (between parallel valleys) and f-type (between perpendicular valleys) are calculated for transitions between points of the minima making use of the phonon spectrum reported in [9].

(4) By application of the symmetry selection rules [10], the phonons allowed for g-scattering reduce to the longitudinal optical (LO) and for f-scattering to the longitudinal acoustic (LA) and transverse optical (TO).

(5) 0.16 eV (1900K, LO, g3 mode, between parallel valley); 0.13 eV (1560K, LA, f2 mode); 0.15 eV (1720K, TO, f3 mode)
After benchmark with VORPAL, we conduct MC electron transport for the pyramid base

(Top) Electric fields from LSP simulation inside and near a dielectric DFE pyramid with an average A-K field of 114 kV/cm. Electrons initially locate at the green box.

(Bottom) Electrons’ energy and longitudinal spatial distributions.

External fields in typical experiment setup produce drift-diffusion type transport with bulk and suprathermal electrons within ~0.6 eV.
Energy quantization in NWs:

- Bulk crystal energy dispersion

\[ E(k) = \frac{\hbar^2}{2m^*} \left( k_x^2 + k_y^2 \right) + \frac{\hbar^2 k_z^2}{2m_L} \]

- Energy quantization in NWs:

Envelope wave function & boundary condition:

\[ \Psi_{n\kappa z}(\rho, \Theta, z) = \frac{N_{\kappa n}}{\sqrt{2\pi}l_z} J_n(\kappa_{\alpha} R_o) e^{ik_z z + in\Theta} \]

\[ J_n(\kappa_{\alpha} R_o) = 0 \]

Energy dispersion:

\[ E_{n\alpha}(k_z) = \frac{\hbar^2 \kappa^2_{n\alpha}}{2m^*_T} + \frac{\hbar^2 k_z^2}{2m_L} \]
Matching boundary conditions with the central region (building the transfer matrix) determines:
- reflection amplitude $r_{\alpha\alpha'}$
- transmission amplitude $t_{\alpha\gamma}$

Evaluate the scattering operator matrix elements:
- back scattering: $\langle -k^L_{\alpha'} | \hat{T} | k^L_{\alpha} \rangle = \frac{i\hbar^2 k^L_{\alpha'}}{m^L_{\gamma} l_c} r_{\alpha\alpha'}$
- forward scattering: $\langle k^R_{\gamma} | \hat{T} | k^L_{\alpha} \rangle = \frac{i\hbar^2 k^R_{\gamma}}{m^*_{\gamma} l_c} t_{\alpha\gamma}$
Evaluation of scattering rates

- Employ Fermi Golden Rule to evaluate:
  - forward scattering rate: \( W^{L,R}_{\alpha,\gamma} = \frac{2\pi}{\hbar} \left| \langle k_R^L(E^L_\alpha) | \hat{T} | k^L_\alpha(E^L_\alpha) \rangle \right|^2 \delta(E_\gamma - E^L_\alpha) \)
  - back scattering rate: \( W^{L,L}_{\alpha,\alpha'} = \frac{2\pi}{\hbar} \left| \langle -k^L_{\alpha'}(E^L_\alpha) | \hat{T} | k^L_\alpha(E^L_\alpha) \rangle \right|^2 \delta(E^L_{\alpha'} - E^L_\alpha) \)

- Modeling scattering rates for:
  - segment radii \( \rho_L, \rho_C, \rho_R = \{5.0 \text{ nm}, 4.5 \text{ nm}, 4.0 \text{ nm} \} \)
  - scattering segment length \( l_c = 1.0 \text{ nm} \)
  - electron in L-segment in subband \( \alpha = 5 \) with kinetic energy \( E_z = \frac{\hbar^2 k_z^2}{2m^*_r} \)