Modeling Secondary Electron Generation and Charge Transport in Diamond with VORPAL

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• Motivation
• Diamond amplifier concept & types of experiments
• Models being developed in VORPAL to simulate diamond amplifier physics
• Results
  – Secondary electron generation
  – Charge transport & electron-hole cloud evolution
  – First simulations on secondary electron gain
• Summary

Motivation

• A new diamond-amplified electron emitter was proposed recently as promising source for generation of high-current, high-brightness 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 emitters.

• Exploration of relevant parameters via computer simulations are expected to provide valuable feedback in the process of designing efficient diamond-amplified electron sources.
Overall Experimental 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

- Our goal is to model and simulate the relevant diamond physics.
Transmission and Emission Type of Experiments are Considered

- Models we have currently implemented in VORPAL allow us to simulate specific properties of the DC transmission experiment.

DC Transmission Experiment
diagram courtesy of Qiong Wu and Chang Xiangyun

DC Emission Experiment

- Modeling of electron emission from diamond surfaces with VORPAL is still to be implemented in future development.

What modeling capabilities are needed?

• To enable end-to-end simulations of diamond-amplified electron emitters we are implementing algorithms to model:
  – Inelastic scattering of electrons (primary & secondary) and holes for generation of electron-hole (e-h) pairs
  – Elastic scattering
    • near diamond surfaces
    • due to ionized impurities
  – Inelastic scattering with phonons
  – e-h recombination
  – Electron emission from diamond surfaces with different electron affinities
• The probability for an electron with kinetic energy $E$ to travel a time $t$ inside the diamond without experiencing a collision is modelled by an exponential distribution.

• The Monte Carlo algorithm supports null collisions.

• The total scattering rate is determined by the scattering rates of the involved collision processes.

• The Monte Carlo algorithm implemented is general. It allows the simulation of any number of scattering processes for which scattering rates, particle energy, and momentum changes can be calculated.

Secondary electron-hole generation


- Both, electrons and holes with $E_{\text{kin}} > E_G$ (5.47 eV) can generate electron-hole pairs.
Scattering cross sections during electron-hole generation

- We used the elastic and inelastic (for secondary electron generation) total cross section from

- Mean free times, paths, and scattering rates are calculated using the total scattering cross sections.
Elastic, inelastic, and total scattering rates during electron-hole generation

- Electrons with energies greater than but close to \( E_G \) (5.47 eV) scatter essentially only elastically.
- For \( E > 100 \) eV, the rates for elastic and inelastic scattering are comparable.

\[
\frac{1}{\tau(E)} = \frac{1}{\tau_{el}(E)} + \frac{1}{\tau_{in}(E)}
\]
• We implemented two models for elastic scattering.
  • Isotropic
  • Anisotropic, small angle scattering, based on the Conwell-Weisskopf approach applicable to, e.g., ionized impurity scattering (Lundstrom, 2000).

• A more accurate calculation of the scattering rates based on a quantum mechanical description is considered for a future development.
Modeling of secondary electron generation

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

$$p(\omega | E) = \frac{\int_{q_-}^{q_+} \frac{\partial^2 \sigma_{in}(q', \omega, E)}{\partial q' \partial \omega} dq'}{\int_{\omega_{\text{min}}}^{\omega_{\text{max}}} \int_{q_-}^{q_+} \frac{\partial^2 \sigma_{in}(q', \omega', E)}{\partial q' \partial \omega'} dq' d\omega'}$$

$$q_{\pm} = k (1 \pm \sqrt{1 - (\omega/E)})$$

obtained from the doubly differential inelastic cross section:

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

- $q$ is the magnitude of the scattered electron’s momentum change, $\epsilon$ is the dielectric function for diamond, and the imaginary part is the energy loss function (ELF).
We sample q-values from the PDF for inelastic scattering.

Probability distribution function:

\[
p(q | \omega, E) = \frac{\partial^2 \sigma_{in}(q | \omega, E)}{\partial q \partial \omega} \int_{q_-}^{q_+} \frac{\partial^2 \sigma_{in}(q' | \omega, E)}{\partial q' \partial \omega} dq',
\]

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

\[
\text{Im} \left(-\epsilon^{-1}(q, \omega)\right) = \frac{1}{\omega} \int_{0}^{\infty} \omega' \text{Im} \left(-\frac{1}{\epsilon^{\text{EXP}}(0, \omega')}\right) f(\omega', q, \omega) d\omega',
\]

in the one-pole approximation for the Lindhard dielectric function:

\[
\text{Im} \left(-\epsilon^{-1}(q, \omega)\right) = \frac{\omega - \hbar q^2 / 2m}{\omega} \text{Im} \left(-\frac{1}{\epsilon^{\text{EXP}}(0, \omega - \hbar q^2 / 2m)}\right).
\]
Energy Loss Function

- Optical data for diamond is used to calculate the ELF.
A comparison of the numerically calculated $p(\omega | E)$ with the distribution obtained from the rejection algorithm (using 100000 samples) verifies the implementation of the algorithm. The pdf is calculated for an initial energy of $E = 1 \text{ keV}$ of the primary electron. The mode of the pdf is close to 33 eV for this value of $E$. 

Momentum change sampling for inelastic scattering

• 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:

\[
p(q \mid \omega, E) = \frac{\partial^2 \sigma_{in}(q, \omega, E)}{\partial q \partial \omega} \int_{q^-}^{q^+} \frac{\partial^2 \sigma_{in}(q', \omega, E)}{\partial q' \partial \omega} dq'
\]

To support conservation of momentum for independently chosen \( E \) and \( \omega \) values, \( q \) must satisfy:

\[|p_{e,s}^i - p_{e,s}^f| < q < |p_{e,s}^i| + |p_{e,s}^f|\]

• From \( E \), the sampled \( \omega \) and \( q \), conservation of energy and momentum, the final momenta of the participating particles can be determined.
Momentum Change Sampling

- The PDF for the momentum change depends strongly on the initial E and the chosen energy change $\omega$. 

The average number of secondary electrons produced for four different initial energies (above $E_C$) of primary electrons & two limiting cases: no loss to the lattice (blue symbols), and with energy loss to the lattice (red symbols).
Evolution of e-h pair generation can be obtained vs primary electron energies.

The generation of secondary electrons has practically completed 100 fs after the primary electron enters the diamond. The total number of generated electrons depends on the primary electron’s input energy and shows some variation among different proposed models.
Energy relaxation vs time due to secondary electron generation

- Simulations allows us to determine the distribution of electron energies after a primary electron enters diamond.
- For a primary e- with initial energy of 1 keV, there are electrons with over 80 eV after 1 fs, for both without energy loss to the lattice (magenta) and with.

Without phonon scattering, secondary electron energies can relax only to $E_G$

- After 10 fs, most of the electrons have energies less than 30 eV
- Most of the electrons have energies within 10 eV after 90 fs.
Approximate representation of e-energy bands for el-ph scattering

- We implemented models for el-phonon scattering for parabolic and non-parabolic conduction bands with spherical and ellipsoidal constant energy surfaces (Jacoboni & L. Reggiani, Rev. Mod. Phys. (1983)).

- For diamond, bands are modeled as parabolic and ellipsoidal.
Band structure and phonon energies of diamond

- The models for el-ph scattering in diamond from Jacoboni & L. Reggiani are based on key features from the full electron band structure and the phonon energies in the (first) Brillouin zone.
We implemented a many-valley model for el-ph scattering in diamond.

- Electron transitions between parallel and perpendicular valleys in el-ph processes are possible in inter-valley scattering.
- The different effective masses along the different axes in k-space are handled using the Herring and Vogt transformation.


Fig. 137. The many-valley model, and the types of scattering process.
Specific types of el-ph scattering implemented for diamond

- Electron intra-valley *inelastic* scattering with acoustic phonons:
  - emission & absorption of phonons with energies (for diamond) in the range $0 < E_{\text{phonon}} < 0.12$ eV

- Electron inter-valley scattering is simulated with three different phonons with energies:
  - 0.16 eV (longitudinal optical, g3 mode, between parallel valley)
  - 0.13 eV (longitudinal acoustic, f2 mode)
  - 0.15 eV (transverse optical, f3 mode)
  - The f# modes are for scattering between perpendicular valleys
  - these processes have similar probability rates so all are important to take into account
Acoustic intra valley el-ph scattering

- The max rate for acoustic intra valley el-ph scattering, $\sim 8 \times 10^{13}$ 1/s, is about two orders of magnitude smaller than the rate for elastic scattering and inelastic (for el-hole creation) for $E > 80$ eV.

- The rate is comparable to the rate for inelastic rate for el-hole generation for $E < 10$ eV.
The rates for inter valley el-ph scattering, max \( \sim 10^{13} \) 1/s, are similar for \( f_2, f_3, \) and \( g_3 \) processes (only for \( g_3 \) shown) and in similar range as the rates for intra-valley scattering.

Since el-hole generation is practically complete after \( \sim 100 \) fs, the el-ph scattering can be neglected during this time interval.
Electron-charged impurity scattering

- We have implemented el-charged impurity elastic scattering and run initial tests with it.
- Initial calculations show that scattering rates could be comparable to el-ph ones.
Electron transport properties can be calculated from the simulations.

- The ability to model electron-phonon scattering allows us to compute the electron average kinetic energy and drift velocity for different applied electric field magnitudes.
The obtained drift velocities from VORPAL simulations agree well with available experimental data:

Electron relaxation to the drift state

- The low energy electron-phonon inelastic scattering processes mediate the relaxation of primary and secondary electrons and holes to the drift state.

- The drift velocity $v_d$ relaxes to the drift state value in a few ps for 1 MV/m external field, 2.7 keV primary electron. The average is from 20 runs.
At low external fields the electron temperature is close to the lattice $T$.

- For external field of 0.05 MV/m, the average kinetic from:
  \[ <E_{\text{kin}}> = \frac{3k_B T}{2} + m_{\text{eff}}(v_d)^2/2 = 0.039 \text{ eV}, \text{ for } T = 300 \text{ K}. \]

- From VORPAL, $<E_{\text{kin}}> = 0.041 \text{ eV}$ with standard deviation of 0.003 eV.
At high external fields, the electrons are in the hot transport regime.

- For $|E| = 1$ MV/m, $<E_{\text{kin}}> = 3k_B T/2 + m_{\text{eff}}(v_d)^2/2 = 0.051$ eV, for $T = 300$ K.
- From VORPAL, $<E_{\text{kin}}> = 0.081$ eV with standard deviation of 0.005 eV. This corresponds to electron temperature $T_e = 530$ K.
Simulations allow us to follow the evolution of system quantities of interest.

The evolution of the electron cloud rms radius enables us to estimate when overlap effect become important for given primary electron beam density and energy.

Following the center of mass of the electron cloud in time confirms that it is in the drift state and moves at the obtained drift velocity (both plots are for 5 MV/m applied electric field).

El-hole cloud expansion has similar behavior as Brownian motion in 3D.

- For a particle in a Brownian motion, $\langle r^2 \rangle$ grows linearly in time for times $t > \tau$, $\tau$ is the effective total scattering time and as $t^2$ for $t < \tau$:

$$\langle r^2 \rangle = C \times t \theta(t - \tau) + A t^2 \theta(\tau - t)$$

- Diagnostics for the long-time el-hole cloud expansion display this behavior.
El-hole cloud expansion – crossover to the linear regime.

- “Early” time results from VORPAL also show the crossover in $<r^2>$

\[
<r^2> = C \times t \theta(t - \tau) + At^2 \theta(\tau - t)
\]

First results on gain per primary e-

- The gain is estimated as number of secondary electrons that are not absorbed at the surface primary electrons enter diamond.
- Due to cloud expansion, e- and holes that reach this surface are removed from the simulation using absorbing boundary conditions.
- Results are for primary electron energy of 2.7 keV.
- Each such electron generated approximately 82 secondary electrons (using Ashley’s model).
- For $|E| = 1$ MV/m, $dx = 0.25 \, \mu m$, 48 e- survive after 4.8 ps.
- For $|E| = 1$ MV/m, $dx = 0.04 \, \mu m$, 56 e- survive after 3.1 ps.
- For $|E| = 0.03$ MV/m, $dx = 0.25 \, \mu m$, 36 e- survive after 4.8 ps.
Electron-hole cloud separation

- Results are for primary electron energy of 2.7 keV.
- For $|E| = 1$ MV/m, $dx = 0.16 \ \mu m$, the el-hole clouds have completed separation at $t = 20$ ps.
  - At $t = 20$ ps, the max Yee E-field magnitude is about an order of magnitude smaller than the external E-field.
- For $|E| = 0.1$ MV/m, $dx = 0.16 \ \mu m$, $t = 20$ ps, about half of the el-hole clouds still overlap.
  - The max Yee E-field magnitude is approximately equal to the magnitude of the external E-field at $t = 20$ ps.
- For $|E| = 0.03$ MV/m, $dx = 0.16 \ \mu m$, $t = 20$ ps, the el-hole clouds are still almost completely overlapping.
  - At $t = 20$ ps, the max Yee E-field magnitude is close to an order of magnitude larger than the external field.
The Debye length was calculated for spherical shells at different distances from the center of electron cloud and at different simulation times.

Cell size of 0.04 μm resolves the observed Debye lengths for times greater than 20 fs and shells at distances larger than 0.2 μm.
Charged impurity scattering effects.

- Comparison of results from a run with charged impurity scattering included to a run without it show (the external field was set to $|E| = 0.1$ MV/m):
  - $v_d = 1.69 \times 10^4$ m/s, $s_v = 0.65 \times 10^4$ m/s has decreased vs the $v_d = 2.06 \times 10^4$ m/s, $s_v = 0.76 \times 10^4$ m/s
  - faster cloud size expansion
  - the separation of the el-hole clouds is slower due to the larger overlap from the faster expanding clouds
  - these result are with representative values for the free electron density $n_0 = 8 \times 10^{14}$ cm$^{-3}$ and the charged impurity density $n_{CI} = 10^{13}$ cm$^{-3}$.
Dielectric constant effects.

- Initial simulations taking into account the dielectric constant of diamond are done via a charge & mass scaling.

- Results with the dielectric constant of diamond (5.7) vs the ones with a unity dielectric constant show:
  - $<E_k> = 0.048$ eV, $\sigma_E = 0.0011$ vs $0.049$ eV, $\sigma_E = 0.0013$
  - $v_d = 1.94 \times 10^4$ m/s, $\sigma_v = 0.43 \times 10^4$ m/s vs $v_d = 2.06 \times 10^4$ m/s, $\sigma_v = 0.76 \times 10^4$ m/s
  - Electron cloud expands somewhat faster in time (due to smaller attraction between the el. and hole clouds
  - The observed Yee E-fields are between 2-3 times smaller
  - Testing of simulations with the dielectric constant is still to be completed.
Summary & Future Work

- 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
  - Test the implementation of charge impurity scattering and study its effects for different impurity densities
  - The effects of fully taking into account the space-charge effects by solving Maxwell equations with VORPAL

- Future code development and simulations work:
  - Implement electron-hole recombination and consider its effects on charge transport
  - Implement a model for electron emission from diamond surfaces with different electron affinities