

MODELING AND SIMULATIONS OF ELECTRON EMISSION FROM DIAMOND-AMPLIFIED CATHODES*

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Abstract

Emission of electrons from a diamond-amplified cathode was recently demonstrated [1]. This experiment was based on a promising new concept [2] for generation of high-current, high-brightness, and low thermal emittance electron beams. The measurements from transmission and emission experiments have shown the potential to realize the diamond-amplified cathode concept. However, the results indicate that the involved physical properties should be understood in greater detail to build diamond cathodes with optical properties. We have already made progress in understanding the secondary electron generation and charge transport in diamond with the models we implemented in the VORPAL computational framework. We have been implementing models for electron emission from diamond and will present results from 3D VORPAL simulations with the integrated capabilities on generating electrons and holes, initiated by energetic primary electrons, propagation of the charge clouds, and then the emission of electrons into diamond. We will discuss simulation results on the dependence of the electron emission on diamond surface properties.

INTRODUCTION

High-average current and high-brightness electron beams are needed in advanced applications such as ultra-high Free-Electron Lasers, electron cooling of hadron accelerators, and Energy-Recovery Linac light sources. To address the high requirements in these applications, a new design for a photoinjector with a diamond amplifier was proposed [2] and is currently being actively investigated (see, e.g., [1] and references therein).

The new photoinjector concept has important advantages [2] (such as the ability to generate high-average current, high-brightness electron beams while providing a very long life time) compared to existing metallic and semiconductor photocathodes. The idea of its operation is to first generate a primary beam of electrons (accelerated to about 10 keV) using a conventional photocathode and inject them into diamond. The energetic primary electrons scatter inelastically in diamond, generating secondary electrons. These electrons, and their related holes, relax their energies initially by producing more electron-hole pairs. When the energy of these free charge carriers reaches close

to the energy gap of diamond, further relaxation of their energy is dominated by scattering with phonons.

In applied electric field, the generated electron and hole clouds drift in opposite directions and are separated. The secondary electrons are transported towards a diamond surface with a negative electron affinity (NEA). Part of these electrons are then emitted into the accelerating cavity of an electron gun. The NEA is used to enhance the emission. Hydrogenation of diamond produces surfaces with NEA. Over two orders of magnitude charge amplification (number of generated secondary electrons emitted relative to the number of primary electrons used as input) could potentially be achieved [1] using this approach.

Investigation of the phenomena involved in using diamond for generation of amplified electron beams via simulations requires modeling of secondary electron generation, charge transport, and electron emission. In previous studies ([3] and references therein), we investigated how to model secondary electron generation and charge transport in diamond. Here, we consider for the first time the emission of electrons from diamond with both negative and positive electron affinity (PEA). Moreover, we implemented a model for band bending near the diamond emission surface and show that this effect is important to take into account.

SIMULATION MODELS

A simplified energy band structure of diamond near a surface with negative electron affinity is shown in Fig. 1 (together with a representation of the processes involved in generating free charges and emitting electrons). First, creation of (secondary) electrons in the conduction band and holes in the valence band is started by inelastic scattering with highly energetic primary electrons. Next, the free electrons and holes relax their energies via inelastic scattering (creating more e-h pairs and/or emission/absorption of phonons). The electrons drift (due to applied field) towards the hydrogenated negative electron affinity surface. In the final step, the electrons are emitted or reflected when they reach the surface. We model emission from surfaces with different electron affinities by implementing code for the propagation of conduction band electrons in a stair-step potential: $V(x, y, z) = 0$, for $x < 0$ and $V(x, y, z) = \chi(y, z)$ for $x > 0$ with the diamond surface set at $x = 0$ and $\chi(y, z)$ is the surface varying electron affinity (measured with respect to the bulk-like bottom of the conduction band at the surface). This is a starting choice for including the electron affinity in the emission since for a constant change in the potential, the problem

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can be solved quantum mechanically giving both the probability for emission and reflection from the surface.

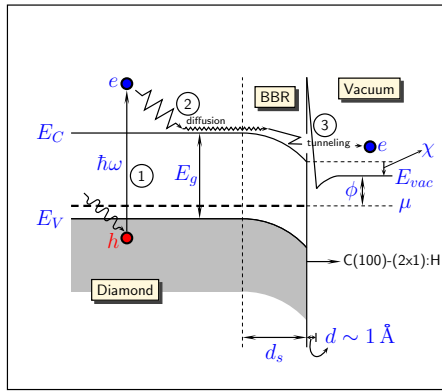


Figure 1: Simplified representation of the processes involved in emitting electrons from diamond.

A more detailed treatment of the surface potential was proposed by Orlov *et al.* [4]. They included a potential barrier (schematically shown in Fig. 1) with a width of the size of dipole layer in which the electron affinity drops from the clean surface value to the negative electron affinity value.

For the stair-step potential we consider here, the probability for emission is given by

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

where E is the kinetic energy of the conduction band electron (also measured with respect to the same level as χ) and α is the angle between the momentum of the electron and the normal to the diamond surface. Note that this formula can be used for emission from both negative and positive electron affinity regions provided $E > \chi$. The dependence of the emission probability on E and α for a case with NEA and one with PEA is shown in Fig. 2. As expected, for NEA the probability for emission approaches unity quickly when E increases above zero and when α decreases below $\pi/2$. For PEA of $\chi = 0.5$ eV, there is a significant region of energies and angles for which electrons are reflected.

The angle of refraction of the emitted electron is $\sin \beta = \sqrt{E/(E - \chi)} \sin \alpha$ with β is also measured with respect to the normal to the surface. The amplitude of the emitted electron's momentum is given by $\sqrt{2m_e(E - \chi)}$.

We consider the band-bending region by introducing an additional field in the simulation confined within a region of the emission surface. The depth of this band bending region has been estimated from experiments [5] (and references therein) to be of the order of $0.1 \mu\text{m}$ with the magnitude of the band bending approximately equal to 0.36 eV. We implemented the models for emission using the stair-step potential and the effect of band-bending region in the VORPAL particle in-cell code.

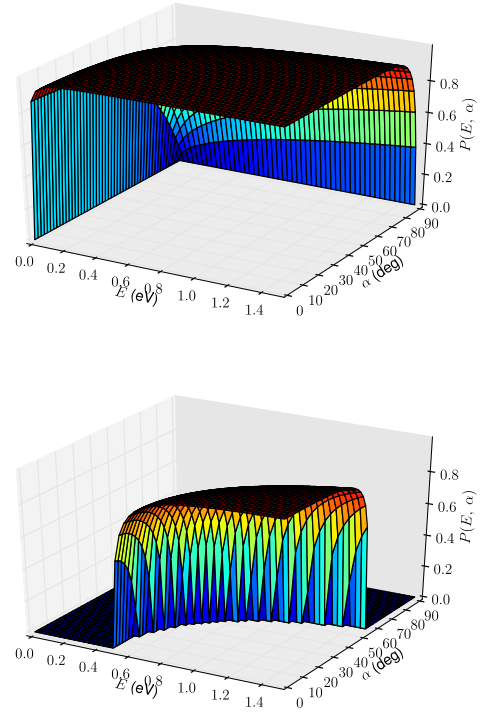


Figure 2: Dependence of the probability for emission, Eq. (1), on E and angle of incidence. The top plot is for $\chi = -0.1$ eV (NEA) and the bottom for $\chi = 0.5$ eV (PEA).

RESULTS

We present results from small-scale VORPAL simulations to start investigating electron emission from diamond and band bending effects. The simulation domain has lengths of $0.63 \times 3.67 \times 3.67 \mu\text{m}$ (with cell lengths of $0.0124 \times 0.1183 \times 0.1183 \mu\text{m}$, $51 \times 31 \times 31$ total number of cells) along the x , y , and z axes, respectively. This domain consists of diamond with length (along x) of $0.6 \mu\text{m}$ followed by a vacuum region of $0.03 \mu\text{m}$. Following the approach in the diamond emission mode experiments [1], we set up the simulations to maintain a given potential difference along the (x) length of the simulation domain using the feedback capability in VORPAL. We selected a potential difference such that the applied field in vacuum is 5 MV/m and in diamond is 0.88 MV/m (the dielectric constant of diamond is approximately 5.7).

The simulations proceed in 3 phases. First, we run for 6000 time steps to establish the desired potential difference across the diamond-vacuum simulation domain. We model diamond as a scalar dielectric using VORPAL's multi-field dielectric updater. In the second phase, we introduce a few (3 to 5) 2.7 keV primary electrons from the left boundary of the simulation domain (at x_{min}) that start to produce secondary electrons and holes. This phase continues for about 1 ps leading to around 700 to 1000 total electrons. We use a time step of 8.3×10^{-17} s to resolve the impact ioniza-

tion scattering rate in this phase. After secondary electron generation completes, we dump the simulation state and restore to execute the third, charge-transport, phase. This phase is dominated by electron-phonon and hole-phonon scattering. The first and third stages are run with a time step of 3.7×10^{-17} s. During the third phase, electrons

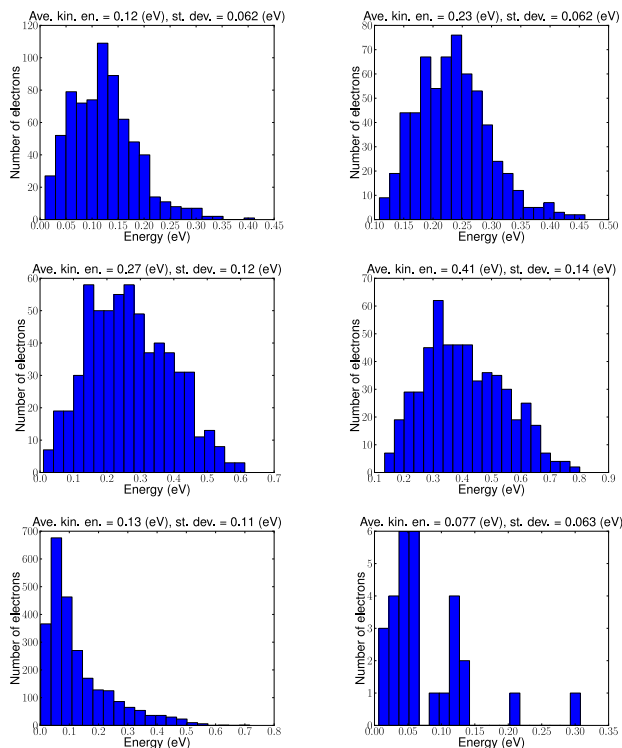


Figure 3: Energy distribution of electrons crossing two surfaces at given x locations (see text) for three different simulation cases. The top row plots are for NEA of $\chi = -0.1$ eV and no band bending. The middle row adds band bending and the bottom row is for PEA of $\chi = 0.5$ eV and band bending.

drift towards the vacuum region under the applied field while holes move to the opposite diamond surface and are extracted from the simulation when they cross it. We considered how electron affinity and band bending affect electrons near the diamond emission surface by measuring electron energy spread at different surfaces (with constant x values). In Fig. 3, we plot such energy histograms for one surface in diamond that is approximately one cell before the emission surface (left column of plots) and for the energies with which the electrons are emitted in vacuum (right column of plots).

Without band bending and with NEA of $\chi = -0.1$ eV (top two plots), the electrons reach the diamond emission surface (top left plot) with average kinetic energy $\langle E_k \rangle$ of 0.12 eV that is essentially equal to their $\langle E_k \rangle$ in bulk diamond (0.11 eV in these simulations). When emitted, their $\langle E_k \rangle$ is 0.23 eV (top right plot). This increase is consistent with the $\chi = -0.1$ eV NEA used.

Beam Dynamics and EM Fields

Dynamics 05: Code Development and Simulation Techniques

The two middle plots are for the same simulation with band bending turned on. The $\langle E_k \rangle$ at the last cell before emission has now increased to 0.27 eV. Note that the max increase could be 0.36 eV but electrons also emit optical phonons while moving in the band bending region. After emission, their $\langle E_k \rangle$ increases to 0.41 eV which is somewhat higher than the magnitude of the NEA but within one standard deviation of it.

In the bottom plots, we plot results from a simulation with band bending and PEA of $\chi = 0.5$ eV. Note that there are many more electrons in the energy histogram that is one cell before the emission surface in diamond (bottom left). This is due to the high number of electrons that are frequently reflected at the emission surface. These electrons cross the history surface diagnostic multiple times and are recorded every time they cross. Since they do not have sufficient energy to be emitted, they are accumulated near the surface. Only a small number of electrons are emitted (bottom right plot) and their $\langle E_k \rangle$ is now decreased to 0.077 eV. These results are consistent with the set values for electron affinity and band bending parameters.

SUMMARY

We reported here initial results from VORPAL simulations on electron emission from diamond. The simulations are based on algorithms we recently prototyped to model electron emission, band bending, negative and positive electron affinity. The results from these simulations confirm that it is of importance to include all of these effects when investigating electron emission from diamond. In a future study, we will additionally consider surface roughness effects and how well results from simulations with these models compare to available experimental data.

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