

INVESTIGATION OF CHARGE GAIN IN DIAMOND ELECTRON BEAM AMPLIFIERS VIA 3D SIMULATIONS*

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Abstract

A promising new concept of a diamond amplified photocathode for generation of high-current, high-brightness, and low thermal emittance electron beams was recently proposed [1] and is currently under active development. To better understand the different effects involved in the generation of electron beams from diamond, we have been developing models (within the VORPAL computational framework) to simulate secondary electron generation and charge transport. The currently implemented models include inelastic scattering of electrons and holes for generation of electron-hole pairs, elastic, phonon, and charge impurity scattering. We will present results from 3D VORPAL simulations with these capabilities on charge gain as a function of primary electron energy and applied electric field. Moreover, we consider effects of electron and hole cloud expansion (initiated by primary electrons) and separation in a surface domain of diamond.

INTRODUCTION

To address the need for high average-current, high brightness electron beams in current and future accelerator-based systems (e.g. electron cooling of hadron accelerators, energy-recovery linac light sources, and ultra-high power free electron lasers), a new design for a photoinjector with a diamond amplifier was proposed [1] and is under active development [2].

This new photoinjector concept has important advantages [1] compared to existing metallic and semi-conductor photocathodes. The idea of its operation is to first generate a primary electron beam using a conventional photocathode and inject it into diamond. The primary electrons scatter in the diamond, generating a cascade of secondary electrons. More recently, highly energetic photons are also being considered in experiments as a source for generation of secondary electrons in diamond instead of using a beam of primary electrons. The secondary electrons drift through the diamond under the acceleration of an applied electric field. The transported, large number of secondary electrons (compared to the number of primaries) are emitted from a diamond surface with a negative electron affinity (NEA) into the accelerating cavity of an electron gun.

We have been implementing models [4] (and our other paper in this proceedings), within the VORPAL [3] computational framework, for simulation of secondary electron

generation and charge transport in diamond in order to better understand the phenomena involved in electron amplification and emission from diamond. Here, we report results on gain when we consider only the loss of electrons due to the electron cloud expansion near the diamond surface where primary electrons enter. Moreover, we compare simulation results with results from experiments [2] on electron gain when using primary electrons to generate the secondaries.

SIMULATION MODELS

When a primary electron with sufficiently high energy enters into diamond, it can experience inelastic scattering leading to losing part of its energy to create electron-hole (e-h) pairs. Moreover, some of the secondary electrons and the related holes are created with large enough energies to also undergo such inelastic scattering and create additional e-h pairs.

Generally, these inelastic processes continue until the free charge carriers (electrons in the conduction band and holes in valance band) in diamond no longer have enough energy to cause the transition of electrons from the valance to the conduction band. The minimum energy for such transitions is equal to the energy gap in diamond, $E_G = 5.46$ eV at room temperature. However, the mean free time between such inelastic scattering events (it can be obtain from the total cross section for this process [5, 4]) increases towards infinity when the energy of the charge carrier decreases towards E_G . Effectively, when the energy of the free carriers is close to 10 eV, the further relaxation of the electrons towards the bottom of the conduction band and the holes towards the top of the valance band is due to low-energy inelastic scattering with phonons.

For the results presented here, we used our implementation of the Ashley's model [5] (and the references therein) for the inelastic scattering for secondary electron generation at 300 K (this extends our initial implementation of this model [4] to $T > 0$ K). For the low-energy inelastic scattering with optical and acoustic phonons we implemented Monte Carlo algorithms based on the models given by Jacoboni and Reggiani [6]. We have validated that the electron-phonon scattering implementation leads to electron drift velocities that agree well with band structure calculations and with experimental data [7].

From the time a primary electron enters diamond, the secondary electron generation is close to complete after 200 fs. The code switches electrons and holes to phonon scattering only, once their energy falls below 11 eV during

* We are grateful to the US DoE for supporting this work under the DE-FG02-06ER84509 grant.

the first 400 fs (the simulation starts with a primary entering the diamond surface set at the $x = 0$ side of the simulated domain). This part of the simulations is done with a time step Δt small enough (of the order of 0.01 fs) to resolve the scattering rate of the high-energy carriers. At 400 fs, we dump the simulation state and restart with all charge carriers switched to inelastic scattering with phonons only. These scattering processes have several orders of magnitude larger mean free time which allows selecting a larger time step after the restart (we have used up to $\Delta t = 2$ fs). The cell size was varied in the range from 0.1 to 2 μm . In all simulations, the cell sizes were equal along the x , y and z directions.

We have implemented a general Monte Carlo algorithm to handle all scattering processes. In between scattering events, the particle-in-cell algorithms in VORPAL [3] provide the capabilities to self-consistently move particles interacting with electromagnetic fields.

RESULTS

We estimate gain from the simulations only by counting the number of free (conduction band) electrons that are successfully separated from the domain of the diamond surface near which the secondary electrons are generated. These results can be (at least qualitatively) compared with the gain measured from experiments done in transmission mode [2] (metal contacts on opposite diamond surfaces are used to create an external electric field of up to several MV/m). Primary electrons are injected through one of the metal contact surfaces (set at $x = 0$ in the simulations with the applied field in the x direction). The generated secondary electrons and related holes move in opposite directions due to the applied field but also expand diffusively due to scattering. In the initial stage of the charged cloud evolution some of the electrons will reach into the metal contact (at the $x = 0$ surface) and will be lost from the diamond. The free electrons that are successfully separated from the domain of the generation, drift towards the other metal contact and we count them as the realized gain. The hole cloud also expand diffusively but is effectively drifted towards the metal contact and extracted there. We model this behavior by using a sink boundary condition (bc) at the $x = 0$ side of the simulation box. The primary electrons are started at this side with an initial velocity along the positive x axis.

The initial charged particle generation and evolution is shown in Fig. 1 at four times after the primary electron enters the diamond at $t = 0$. Only the domain near the expanding clouds (created by 5 primary electrons from independent runs with a single primary electron each) is shown. The gain results are from averages of 48 such runs with the deviations used to calculate errors. Primary electrons in the experiments are estimated to create effectively independent charge clouds. The distribution of particles at 200 fs confirms that at earlier times, when the particles are created, the electron and hole clouds effectively overlap.

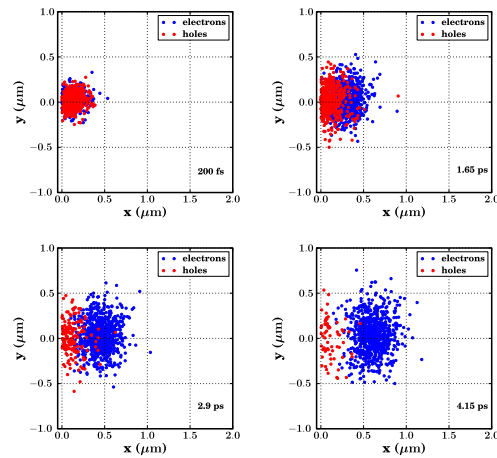


Figure 1: The expansion of secondary electron and hole clouds created by a primary electron with 2.7 keV energy (entering a diamond surface at $x = 0$) in an external fields of 3 MV/m shows the electron cloud has drifted away from the surface after 4 ps.

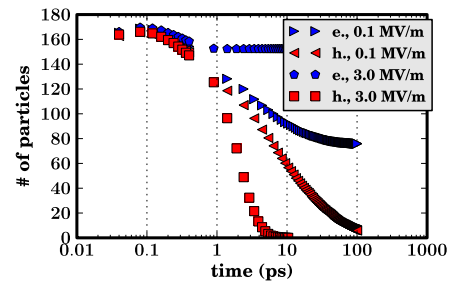


Figure 2: The evolution of the electron and hole numbers vs time, for 0.1 and 3 MV/m fields, indicates how the gain depends on the field amplitude and the time scales for reaching saturation.

For 3 MV/m field and at $t = 4.15$ ps, the (gained) electrons have effectively separated from the surface and from the hole cloud. The small number of holes present in the simulation at this time shows that most of the holes have already recombined at the metal contact. This behavior is explicitly confirmed by considering the evolution of the number of electrons and holes vs time, shown in Fig. 2 for 3 MV/m field (same as in Fig. 1) and for 0.1 MV/m. As expected, the rate at which electrons drift away from the diamond surface increases when increasing the field. The less amount of time the electrons are close to the metal contact surface, the less number of electrons are lost from the diamond, thus leading to higher gain.

We compare gain results from the simulations to experimental data [2] for primary electron energies of 0.7, 1.7, 2.7, 3.7, and 4.7 keV in Fig. 3. The simulations show the same overall dependence on the applied field as the experiments. The results from the simulations and the experiments are in very good agreement for the 2.7 keV case and

are close at the lower energies. However, for the 3.7 and 4.7 keV cases, the simulations predict 16 and 25 % higher gain than observed in the experiments.

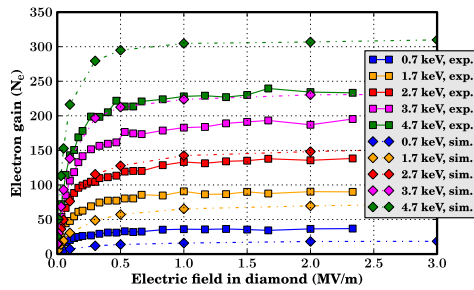


Figure 3: Comparison of the electron gain from transmission experiments [2] with the simulations shows the same behavior for different primary electron energies and fields.

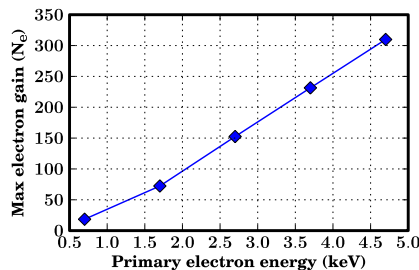


Figure 4: The maximum number of electrons in the drifted clouds indicates two orders of magnitude gain for primary electron energy larger than 2.5 keV.

The higher gain seen in the simulations for these two cases could potentially be due to two reasons. In the simulations, the gain was determined by the number of electrons that are successfully separated from the metal contacts at diamond surface near which the generation happens. Any additional electron loss during the propagation to the other metal contact is not taken into account (e.g., due to trapping or recombination with holes in diamond). However, the gain from the experiments is determined by the total transmitted charge collected at the opposite metal contact. Secondly, the gain in the experiments was determined [2] assuming that the primary electrons lose a constant amount of energy when going through the metal contacts before entering in diamond. However, this loss is generally dependent on the energy of the particles.

The dependence of the maximum gain on the primary electron energy in the simulations, shown in Fig. 4, indicates that at higher energies, the diffusive motion does not affect the gain as much as at lower energies. For a 4.7 keV primary electron, the average energy to generate a secondary electrons is about 15 eV, while for a 700 eV primary electron, it is 38 eV. Note that simulations started with a primary electron in bulk diamond using with this model for the inelastic scattering show about 14 eV average energy

to generate an electron-hole pair. This value is within the range from 10 to 17 eV reported [5] previously by different experimental, theoretical, and computational studies.

SUMMARY

We reported here initial simulation results on charge gain from diamond that indicate the gain can be optimized by increasing the primary electron energy and the magnitude of the applied electric field. However, increasing the field will lead to increasing the effective temperature of the drifting electrons (the regime of hot electron transport) potentially increasing the thermal emittance of the emitted beam. At the intermediate primary electron energies considered, the gain from the simulations agrees very well with experimental data. At the higher energies, the simulations predict larger gain than the experiments. However, in the simulations we have considered only loss due to the diffusive motion near the diamond surface where secondary electrons are generated. In the future, we will investigate the complete transmission process, including effects of trapping and collection of the electrons at the second metal contact. We are also implementing a more accurate model for the secondary electron generation and will consider emission from diamond with different electron affinities. Finally, we have started to investigate via simulations secondary electron generation caused by highly energetic photons to better understand results from such experiments.

REFERENCES

- [1] I. Ben-Zvi, X. Chang, P. D. Johnson, J. Kewisch, and T. Rao. Secondary emission enhanced photoinjector. C-AD Accelerator Physics Report C-A/AP/149, BNL, 2004.
- [2] X. Chang, I. Ben-Zvi, A. Burrill, J. Grimes, T. Rao, Z. Segalov, J. Smedley, Q. Wu. Recent Progress on the Diamond Amplified Photo-cathode Experiment. In *PAC07*, IEEE, pp. 2044-6, 2007; X. Chang *et al.*, First Observation of an Electron Beam Emitted from a Diamond Amplified Cathode. In these proceedings.
- [3] C. Nieter and J. R. Cary. VORPAL: a versatile plasma simulation code. *J. Comput. Phys.*, 196:448-473, 2004.
- [4] D. A. Dimitrov, R. Busby, D. L. Bruhwiler, J. R. Cary, I. Ben-Zvi, T. Rao, X. Chang, J. Smedley, Q. Wu. 3D Simulations of Secondary Electron Generation and Transport in a Diamond Amplifier for Photocathodes. In *PAC07*, IEEE, pp. 3555-7, 2007.
- [5] B. Ziaja, R. A. London, and J. Hajdu. Unified model of secondary electron cascades in diamond. *J. Appl. Phys.*, 97:064905-1/9, 2005.
- [6] C. Jacoboni and L. Reggiani. The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials. *Rev. Mod. Phys.*, 64:645-705, 1983.
- [7] T. Watanabe, T. Teraji, T. Ito, Y. Kamakura, and K. Taniguchi. Monte Carlo simulations of electron transport properties of diamond in high electric fields using full band structure. *J. Appl. Phys.* 95:4866-74, 2004.