MONTE CARLO SIMULATIONS OF CHARGE TRANSPORT AND ELECTRON EMISSION FROM GaAs PHOTOCATHODES*

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Abstract

The need for a bright electron beam is increasing in the fields of x-ray science, electron diffraction and electron microscopy which are required for colliders. GaAs-based photocathodes have the potential to produce high-brightness, unpolarized and polarized, electron beams with performance that meets modern collider requirements. Even after decades of investigation, however, the exact mechanism of electron emission from GaAs is not well understood. Therefore, we investigate photoemission from a GaAs photocathode using detailed Monte Carlo electron transport simulations. Instead of a simple stepwise potential, we consider a triangular barrier including the effect of the image charge to take into account the effect of the applied field on the emission probability. The simulation results are compared with the experimental results for quantum efficiency and energy distributions of emitted electrons without the assumption of any ad hoc parameters.

INTRODUCTION

The successful operation of X-ray light sources, free electron laser (FEL), and linear accelerator facilities depends on providing reliable photocathodes [1] for generation of low emittance, high-brightness electron beams using conventional lasers.

An ideal photocathode must have a high quantum efficiency (QE), low mean transverse energy (MTE), a quick response time and a good operational lifetime. GaAs-based photocathodes have been experimentally tested and shown [2] to have the potential to produce high-brightness unpolarized and polarized, electron beams with performance (e.g., high QE and low emittance) that meets FEL and modern collider requirements. A better understanding of the physics of photoemission in GaAs will open new possibilities for creating very low emittance high efficiency photoemitters.

However, there are still a number of issues [3] to solve in order to develop an optimized photocathode design. It is of interest to better understand the quantum efficiency and energy distribution of generated beams as a function of temperature, laser frequency, cathode material, doping concentration, electron affinity, and surface properties (e.g., roughness, band bending, charge trapping).

Accurate simulation capabilities help to optimize the design of a semiconductor photocathode. Three dimensional, particle-in-cell (PIC) codes can accurately simulate the evolution of electron beams for these purposes.

The VSim simulation and modeling framework [4] includes a variety of physical models that make it useful for a broad range of research in plasma physics and computational electrodynamics. It can model a plasma as particles, a fluid, or a particle-fluid hybrid; it can treat electromagnetic fields either self-consistently or in the electrostatic limit; and it provides both explicit and implicit time updates.

In a previous work [5], we investigated effects of charge transport and surface properties on electron emission from GaAs with a specific surface potential. However, it did not include the image charge effect, zero applied field was assumed, and the space-charge field was not included in the models. Here, we have started to consider electron emission properties when the space-charge field is included and the applied field is non-zero. We have done simulations with a surface potential that is often used to investigate electron emission and includes the image charge effect. Finally, we have used a reduced model for the calculation of the electron emission probability that is fast to evaluate but potentially less accurate than the model in Ref. [5].

MODEL

The simulation is based on the three-step model initially proposed by Spicer [6]. The three valley model is used to describe the band structure of GaAs. Here, we briefly describe these models. More detailed explanation can be found in Ref. [5].

Three Step Model

The three-step model takes into account the dependence on photon energy and (implicitly) on temperature. Fig. 1 shows a schematic representation of the three-step model for *p*-doped GaAs photocathode. The creation of electron-hole pairs due to absorption of photons is treated in the first step. A photon with sufficient energy is absorbed by a valence band electron leading to its transition to the conduction band and the formation of a hole in the valence band. The difference between the photon energy and the energy gap of the semiconductor material is transferred into kinetic energy of the created free charge carriers. In the second step, created conduction band electrons undergo different scattering processes and propagate diffusively. Some of these electrons will reach the photocathode surface and be

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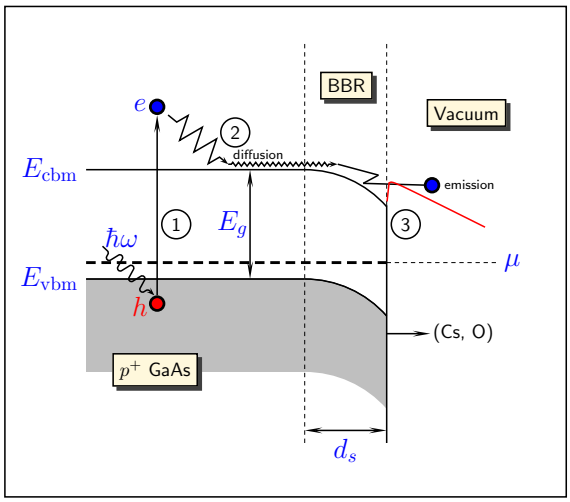

Figure 1: Schematic representation of the three-step model. First, a photon is absorbed causing the generation of an electron-hole pair. Next, the free electron undergoes phonon scattering and diffuses towards the GaAs cesiated electron affinity surface. In the final, third step, a conduction band electron undergoes emission (over barrier or tunneling) or reflection when impinging on the GaAs-vacuum interface.

emitted, during the third step as schematically shown in Figure 1.

Three Valley Model

In our simulation, we use the three valley model of GaAs, which assumes the top 3 valence bands (heave hole, light hole and the split-off) to be spherical and parabolic near the Γ point. The first conduction band is modelled as a combination of three valleys (Γ, L, and X valleys).

Electron-Hole Generation

As light propagates to a distance x in a photocathode (measured from its surface), its intensity decrease is given by the expression

$$I = I_o exp\left(-x/a\left(\hbar\omega\right)\right),$$

where $a\left(\hbar\omega\right)$ is the photon's energy-dependent absorption length. We assume that excitation of electrons from the valence band to the conduction band is the only dominant light absorption process. Doping dependent absorption length is calculated using the model developed by Lao *et al.* [7] The energy w.r.t. the conduction band minimum (CBM) of the electron excited into the Γ valley by a photon is calculated by equating the energy difference between the initial and final state of the electron to the energy of the photon [8].

Conduction Band Electron Transport

The charge transport of free carriers in the presence of applied electric field represents a drift-diffusion process. The simulation tracks electrons excited into the conduction band in both real space and k-space using semi-classical equation of motion. The main problem in modeling charge transport in GaAs is to determine the relevant scattering processes involved, how to calculate their rates as a function of electron energy, and how to determine final wave vectors in each type of scattering process. In this study, we considered impurity, phonon, and carrier-carrier scattering. For impurity scattering, we only consider scattering with charged impurities, because most impurities in GaAs are ionized at room temperatures. For phonon scattering, we consider acoustic, optical, and polar optical phonon scattering processes. Piezoelectric scattering is ignored. Here, we consider only electron-hole scattering (and neglect electron-electron and electron-plasmon processes) since it is the dominant carrier-carrier process for electrons in heavily *p*-doped GaAs. The density of free electrons is very small and plasma oscillations of the holes are heavily damped, therefore, electron-electron and electron-plasmon processes can be neglected.

Modeling Electron Emission

The simulation results we have reported here use the electron emission model developed by K. Jensen [9] with the image charge effect included in the surface potential. The potential energy of an electron in this surface potential is given by

$$V\left(x\right) = \chi - Fx - \frac{Q}{x}, \qquad (1)$$

where χ is the electron affinity (measured relative to the conduction band minimum at the surface), $Q = Q_0\left(K_s - 1\right)/\left(K_s + 1\right)$, $K_s \approx 13$ is the (static) dielectric constant for a GaAs cathode, and $Q_0 = q^2/\left(16\pi\varepsilon_0\right)$ with q the fundamental charge and ε_0 the permittivity of vacuum. The probability of emission is then given by Eq. (18) in Ref. [9] as a function of the electron's effective energy along the direction perpendicular to the emission surface. This approximate model for calculation of the emission probability, due to reducing the problem to one spatial dimension, requires us to extend our algorithm in VSim to explicitly preserve conservation of transverse momentum during emission. In the MATLAB code developed for the study by S. Karkare *et al.* [5], a transfer matrix (TM) approach was used to calculate the emission probability that explicitly takes into account conservation of transverse momentum. The TM method is currently being implemented in VSim and results with it will be presented elsewhere.

COMPARISON TO PHOTOEMISSION EXPERIMENTS

We use VSim with an electromagnetic pusher and include space charge effects. Band bending field and image charge effects are considered too. We also include the effect of an external applied field which was set to 1 MV/m. The values of GaAs parameters used in the simulations are given in Ref. [5]. The band bending region energy was 0.461 eV and its length was 8.4 nm calculated via the approach in Ref. [5]. Three-dimensional simulations are performed with

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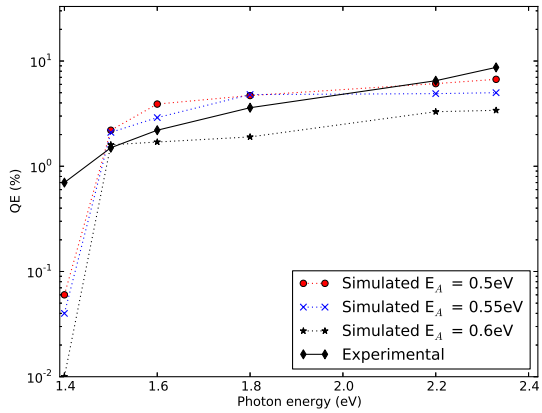

Figure 2: Comparison of measured and simulated spectral response. The electron affinity is an input parameter in the simulations. Results close to the experimental data are obtained for $\chi = 0.55$ eV.

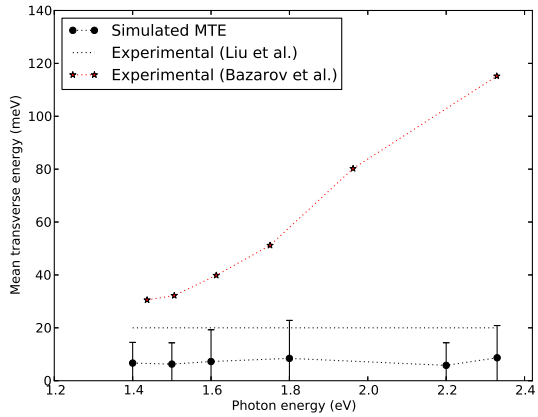

Figure 3: Comparison of measured (Liu *et al.* [10] and Bazarov *et al.* [11]) and simulated MTE using $\chi = 0.55$ eV in our simulations.

$30 \times 30 \times 30$ cells and 1000 electrons except for the lowest photon energy 1.4 eV in which case 10000 electrons were considered. We run simulations to 100 ps to collect data. The electron affinity is measured from the CBM at the GaAs surface (note that some authors consider χ relative to the CBM in bulk).

Spectral Response

Figure 2 shows the spectral response measurement along with the results obtained from the simulation for various values of electron affinity. The simulation results with electron affinity of 0.55 eV are overall closest to the experimental data. It is worth to mention that the simulation results are obtained entirely from the band structure and transport properties of GaAs and no ad-hoc parameters have been used. The only uncertain variable is the electron affinity which is deduced to be 0.55 eV (for the surface potential, Eq. (1), we considered) by comparing the simulated results to the experiment. In order to calculate the quantum efficiency, the reflectivity value of GaAs was taken from Ref. [5].

Mean Transverse Energy

We show MTE results from our simulations in Figure 3 together with data from two experimental measurements [10, 11]. The electron affinity was set to 0.55 eV in the simulations. Our results do not include scattering during emission process, and show very small MTE due to the narrow cone effect similar to the results from the MATLAB code [5]. The MTE deduced from the angular and energy distribution obtained by Liu *et al.* [10], using white light for excitation, is close to the simulation results. However, data from other experiments, including Bazarov *et al.* [11], give larger values outside of the narrow cone prediction. The reason for this discrepancy is still to be understood. Additional scattering during emission through the Cs layer was considered [5] leading to higher MTE values. However, emission dependence on surface roughness, orientation, surface cleanliness, and external electric field effects are still to be investigated in detail.

CONCLUSION

We presented simulation result on charge transport and electron emission from GaAs cathodes. Our model includes effects of applied field and image charge in the surface potential, space-charge fields and band bending. This model can achieve agreement with experimental data on QE with electron affinity the only free parameter varied. However, different surface potentials have been proposed and investigated in other studies [5] (and references therein). Further work is needed to determine the most relevant surface potential and related surface physics models (e.g. roughness and space-charge region in non-equilibrium) that could best describe observed experimental data.

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