

Simulating photoemission performance of a nanostructured alkali photocathode with a three-dimensional coupled finite-difference time domain Monte Carlo technique

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(Received 28 January 2026; accepted 16 June 2026; published 11 August 2026)

We present a methodology for modeling the photoemission process in nanopatterned photocathodes using finite-difference time domain (FDTD) and 3D Monte Carlo (MC) methods adapted for tasks with 3D nanopattern geometry. Using MC, we calculated the electron transport inside the alkali semiconductor. The FDTD method was used to simulate light absorption in a photocathode. This coupled approach self-consistently models resonant effects, electron excitation, transport to the cathode surface, and emission into vacuum. Furthermore, this approach enables the study of two-dimensional (2D) nanopatterned structures. We studied semiconductor photocathodes with 1D and 2D nanopatterned metal substrates. We calculated the quantum efficiency and intrinsic emittance at photon energies from 1.8 to 2.4 eV. We have demonstrated that the quantum efficiency of a nanopatterned photocathode is significantly higher than that of a photocathode with a flat interface. We also demonstrated that the quantum efficiency of a two-dimensional nanostructured photocathode is polarization-independent. At the same time, the cathode intrinsic emittance remains unchanged upon nanopatterning.

DOI: [10.1103/nmfq-j22y](https://doi.org/10.1103/nmfq-j22y)

I. INTRODUCTION

Highly efficient semiconductor photocathodes are crucial components in electron sources [1–5] and in various technologies such as x-ray free electron lasers [6]. Quantum efficiency (QE), defined as the ratio of emitted electrons to incident photons, is a key photocathode parameter. Higher QE enables the use of lower-power lasers, reducing manufacturing costs and mitigating component overheating risks [7,8].

Classical metal photocathodes [4] have a high lifetime, low response time, and do not require high vacuum quality. However, typical QE of a metal photocathode is low (~0.01%–0.001%) [7,9], which requires the use of expensive and powerful lasers to achieve high photocurrents. In contrast, semiconductor photocathodes have significantly higher QE. Particularly, alkali antimonide photocathodes have high QE in the visible spectrum [5], for example, the

QE of K₂CsSb photocathode is approximately 10% [1]. For free electron lasers, a reduction in response time is required. One way to reduce the response time is to reduce the thickness of the cathode layer. This, however, may lead to the decrease of QE [5]. Surface plasmon polaritons (SPPs) offer a potential solution, without compromising response time or QE [5,10]. Simulations indicate that SPPs can significantly increase QE [3–5,11–15].

Most of the plasmon-enhanced photocathodes studied so far rely on purely metallic nanostructures [11–15], whereas the studies of the plasmon-enhanced alkali antimonide photocathodes were mostly restricted to nanostructures with 1D periodicity, which exhibit strong polarization dependence [4,5]. This limits their practical use in applications where the light polarization may vary or remain undefined, such as in electron sources driven by polarization-modulated lasers or in systems utilizing unpolarized or natural light. Polarization-insensitive two-dimensional (2D) grating could overcome this limitation while maintaining high QE through SPP excitation, making it highly desirable for next-generation electron sources in accelerators and advanced light detection systems.

While numerous studies model photoemission from semiconductor photocathodes [1,10], most of them focus on planar structures without nanostructuring. SPPs excitation in nanostructured cathodes alters the internal

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electromagnetic field distribution, profoundly impacting the photocathode performance. Accurately modeling these effects requires sophisticated electromagnetic simulations. Typically, simulating photoemission from nanostructured photocathodes involves a two-step approach: first, electromagnetic modeling determines the photon absorption profile and the subsequent generation rate of excited electrons within the material; second, electron transport within the semiconductor is simulated, using the spatial generation profile from the first step as the initial conditions. To reduce computational costs, various approximations are often employed. For instance, the work by Jiang *et al.* [5] uses a hybrid approach: the light energy absorbed during the initial transmission through the cathode layer is assumed to decay exponentially, while the additional absorption due to surface plasmons is obtained from electromagnetic simulations using CST STUDIO [5]. We acknowledge that the approach used in [5] was well justified for the specific geometry and objectives of that study. For our purposes, however, which involve full 3D nanopatterning and arbitrarily shaped 2D gratings, we found it necessary to adopt a more comprehensive method. Therefore, in the present work, we employ a coupled finite-difference time domain Monte Carlo (FDTD-MC) approach that directly computes the total electromagnetic field distribution from Maxwell's equations without splitting the absorption into separate parts. This allows us to capture the full field distribution self-consistently, which is particularly important for accurately modeling photoemission from the 2D grating structures investigated here.

One of the approaches to modeling electron transport is to solve the diffusion equation [16], but it is applicable only for systems that are large enough in comparison with the free path length. To overcome this limitation, we employ a 3D Monte Carlo transport simulation. We calculate the absorbed photon distribution in the semiconductor layer using the FDTD method and subsequently employ a 3D Monte Carlo technique to simulate electron transport, thereby providing a more rigorous and physically detailed model of the photoemission process from nanostructured photocathodes.

Transport calculations are also frequently performed in a 2D approximation [1,4,5]. While a 2D approximation of the MC transport model reduces computational cost, it fails to capture the full complexity of the three-dimensional plasmonic field distributions and electron trajectories in 3D structures. Our model is a development of the approaches presented in [1,4,5]. We have adapted them to address the photoemission of photocathodes with an arbitrary 3D geometry. We investigate the characteristics of nanopatterned photocathodes with various types of gratings and study the effect of SPP excitation on the QE of a photocathode.

The purpose of this work is to study the effect of SPPs on the photoemission of a photocathode with a

two-dimensional nanostructure. The paper is organized as follows. In Sec. II, we provide a detailed description of our method. The subsequent Sec. III details the simulation results for nanostructured photocathodes with varying grating parameters. Finally, we conclude with a discussion of these results in Sec. IV.

II. METHODOLOGY OF PHOTOEMISSION MODELING

The photoemission process in the photocathode is considered to occur in three stages: absorption of a photon emitted from a source, excitation of an electron, and transport of the charged particle in the semiconductor [17]. The band structure of a semiconductor and the process of electron excitation from the valence band to the conduction band are shown in Fig. 1 E_a —electron affinity, E_g —band gap. QE of the photocathode is equal to the ratio of the number of photoelectrons N_{emission} to the number of photons emitted by the light source N_{ph} :

$$\text{QE}(\hbar\omega) = \frac{N_{\text{emission}}(\hbar\omega)}{N_{\text{ph}}},$$

where $\hbar\omega$ is the photon energy.

The photocathode structure that we study hereafter consists of a semiconductor cathode layer deposited on a thick metal substrate. All nonreflected photons are absorbed in the substrate and semiconductor film. Quantum yield (QY) $J(\hbar\omega)$, which is the ratio of the number of photoelectrons to the number of absorbed photons. $J(\hbar\omega)$ and QE are related by the following relation:

$$\text{QE}(\hbar\omega) = \text{Abs}(\hbar\omega)J(\hbar\omega),$$

where $\text{Abs}(\hbar\omega)$ is the absorption coefficient of the photocathode. The fraction of photons absorbed in some small volume of the photocathode dv near a point with

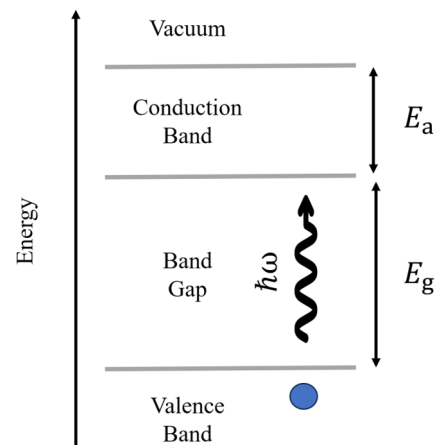


FIG. 1. Band structure of a semiconductor.

coordinates x can be expressed as follows:

$$d\rho_V(\hbar\omega, \mathbf{x}) = \frac{w(\hbar\omega, \mathbf{x})dV}{\int_V w(\hbar\omega, \mathbf{x})dV}. \quad (1)$$

The integration is performed over the entire volume V of the photocathode. Here $w(\hbar\omega, \mathbf{x})$ is the energy density of the electromagnetic field:

$$w(\hbar\omega, \mathbf{x}) = \frac{1}{\omega} \text{Im}(\epsilon(\hbar\omega, \mathbf{x})) \frac{|F(\hbar\omega, \mathbf{x})|^2}{2},$$

where $\epsilon(\hbar\omega)$ is the dielectric constant of the material, $F(\hbar\omega, \mathbf{x})$ is the electric field at point $\mathbf{x}$, and ω is the frequency. When solving Maxwell's equations using the FDTD method, both the absorption of light during its propagation through the semiconductor layer and the additional absorption from localized electromagnetic fields arising from the excitation of SPPs are automatically taken into account. Furthermore, our approach also accounts for the portion of the field energy absorbed in the metal substrate.

We assume that the processes of photon absorption and electron excitation can be considered independently of electron transport within the cathode layer [17]. Let the energy distribution of the excited electrons in the conduction band be described by the function ρ_E , and p_{XE} be the probability of the transport of an electron with energy E from a point $\mathbf{x}$ to the surface with a subsequent emission of this electron out of the semiconductor. Consider absorption of a photon leading to the electron being excited to the conduction level with energy E . The QY of electrons with energy E from a small volume dV at point $\mathbf{x}$ of the semiconductor can be written as follows [16]:

$$dJ(\hbar\omega, E, \mathbf{x}) = \rho_E(E) p_{XE}(\mathbf{x}, E) d\rho_V(\hbar\omega, \mathbf{x}).$$

Let us count the excitation energies from the bottom of the conduction band; then the maximum electron energy in the conduction band is $\hbar\omega - E_g$ and the minimum is 0. Integrating the expression for the QY over the electron energy and photocathode volume, we obtain the final expression for quantum yield:

$$J(\hbar\omega) = \int_V dV \int_0^{\hbar\omega - E_g} \rho_E(E) \rho_V(\mathbf{x}) p_{XE}(\mathbf{x}, E) dE.$$

The problem of calculating QE decouples into two independent tasks: the multiplier Abs can be obtained from the electromagnetic calculation and $J(\hbar\omega)$ from the transport calculation.

In the following, the FDTD method is used as the electromagnetic part of the simulation to calculate the field distribution inside the photocathode and to obtain the absorption coefficient and the fraction of photons absorbed

by the semiconductor. A Monte Carlo simulation, which will be detailed in the next chapter, provides $J(\hbar\omega)$.

III. SIMULATION OF ELECTRON PHOTOEMISSION

To investigate the influence of SPPs on the emission properties of photocathodes with arbitrary 3D nanostructuring, as well as the polarization dependence of these properties, we employ the three-dimensional Monte Carlo simulation method to model the photoemission process. The reliability of describing photoemission within the framework of Spicer's three-step model has been previously confirmed [1,4,5]. A well-established methodology and algorithm for Monte Carlo simulation in the two-dimensional case have been developed [1], and there are also studies on the modeling of the K_2CsSb photocathode with SPPs [5]. In the present work, the simulation approach is based on the aforementioned previous studies; however, the key modification is the extension of the model to a full three-dimensional case. This enables the investigation of photocathodes with 3D nanostructuring and the study of the polarization dependence of emission.

Let us consider the transport of a photoelectron in a semiconductor based on an alkali cathode material (K_2CsSb , Cs_3Sb , Cs_2Te) with a thickness on the order of several electron mean free paths. After excitation by a photon, the electron transitions from the valence band to the conduction band. Within the semiclassical transport model, the motion of the electron is described by its wave vector $\mathbf{k}$, which is related to the electron energy via the material's dispersion law $E(\mathbf{k})$. We use a quadratic approximation of the dispersion relation for the electron. Deviation from the quadratic dispersion law becomes apparent at electron energies below 0.15 eV [18].

In the absence of any other factor exciting electrons, the concentration of electrons in the conduction band will be significantly lower than in the almost completely filled valence band [17]. This implies that, for the most part, electron-electron interaction will only be possible if the electrons have sufficient energy to transition from the valence band to the conduction band. Electron-electron scattering can only occur if an electron possesses energy greater than E_g relative to the bottom of the conduction band [18]. This work considers photon energies on the order of $2E_g$ or less; therefore, the influence of electron-electron scattering can be considered negligible.

Electron-phonon scattering represents the interaction of an electron with crystal lattice vibrations. Scattering can occur on optical or acoustic phonons [2]. The influence of scattering on acoustic phonons can be neglected due to its small magnitude. Scattering on acoustic phonons occurs 25 times less frequently than on optical ones [2]. When scattering on a phonon, the electron abruptly changes its direction of motion [17]. The energy of an optical phonon is very small at room temperature compared to the energy

of the electron, on the order of 0.03 eV [17], but the mean free path in this case is of the order of several nanometers. For a characteristic electron energy of 1 eV, multiple phonon scattering events can occur. Multiple phonon scatterings lead to a diffusive (Brownian) character of electron motion and its energy relaxation toward the bottom of the conduction band or transport to the surface. When an electron scatters off a phonon, it can either gain or lose energy equal to the phonon energy. The ratio of the probability of gaining, W_- , or losing, W_+ , energy is described by the expression [19]:

$$\frac{W_-}{W_+} = \exp \frac{E_{\text{ph}}}{k_B T} \log \frac{1 + \sqrt{1 - \frac{E_{\text{ph}}}{E}}}{1 - \sqrt{1 - \frac{E_{\text{ph}}}{E}}} \left[\log \frac{1 + \sqrt{1 + \frac{E_{\text{ph}}}{E}}}{1 - \sqrt{1 + \frac{E_{\text{ph}}}{E}}} \right]^{-1}.$$

Assuming that the phonon energy E_{ph} is much less than the electron energy ($\frac{E_{\text{ph}}}{E} \rightarrow 0$), we find that the ratio of the probabilities for an electron to lose or gain energy upon scattering by an optical phonon is independent of the electron's energy and is equal to:

$$\frac{W_-}{W_+} \approx \exp \frac{E_{\text{ph}}}{k_B T}.$$

For an electron to be able to leave the semiconductor, several conditions must be met [7]. First, the electron must be located at the semiconductor-vacuum interface. Second, the laws of conservation of momentum and energy must be satisfied during the electron emission. Third, the electron must overcome the potential barrier at the interface.

From the conservation laws of energy and momentum, it follows [1] that an electron can be emitted if the following condition on the angle θ_{in} between its direction of motion and the surface normal is satisfied:

$$\sqrt{\frac{E_a}{E}} > \cos \theta_{\text{in}}.$$

Unlike metals, where the electron transmission probability $D(E)$ can be well approximated by a step function in energy, surfaces with low electron affinity likely present a barrier that is more akin to a triangular shape, albeit one of low height [20]. The probability of an electron emission through the potential barrier for alkali semiconductors is given by

$$D(E) = \frac{4\sqrt{E(E - E_a)}}{(\sqrt{E - E_a} + \sqrt{E})^2}.$$

The Fermi level of the metal is aligned with the Fermi level of the semiconductor, allowing electrons to freely penetrate the metal (Cu, Mo, Cr, Ag) [1]. In metals, electron-electron scattering predominates [9], so an electron loses its energy almost immediately and no longer

participates in the photoemission process. For the same reason, the contribution of the metallic substrate to the photocurrent is extremely small and can be neglected.

To calculate an accurate 3D representation of strong optical field gradients intrinsic to the metallic-based nanostructure, we employed our high-performance software tool “HiFDTD” [21,22], featuring space-temporal blocking for the finite difference mesh update. The obtained 3D distribution of optical fields was used as an input for simulating electron generation in (1).

For the electron transport part of the simulation, we developed a custom 3D MC code to simulate electron transport within the semiconductor, enabling calculation. It allows us to calculate $J(\hbar\omega)$ and the intrinsic emittance.

Transport simulation can be represented in three stages [17]: electron initialization, electron movement, and boundary collision. The last two stages repeat until the termination conditions are met.

Electron initialization is performed according to the energy and coordinate distribution of excited electrons. Six coordinates are assigned to the electron inside the semiconductor: three spatial and three velocity components. The initial density of energy distribution ρ_E of the electrons was determined by the photon energy and the density of electronic states $f(E)$ (DoS), according to:

$$\rho_E(E) dE = \frac{f(E)f(E - \hbar\omega)dE}{\int_0^{\hbar\omega} f(E)f(E - \hbar\omega)dE}.$$

The energy E is counted from the bottom of the conduction band. At the beginning of the simulation, the electron has spatial coordinates generated according to the distribution in (1). The initial direction of the electron velocity was chosen randomly with a uniform distribution. The velocity magnitude is calculated from the initial energy using the following equation:

$$|\mathbf{v}| = \sqrt{\frac{2E}{m_{\text{eff}}}},$$

where m_{eff} —effective mass of an electron.

The next stage is the electron transport. At this stage, the electron moves in the volume of the semiconductor, being randomly scattered by phonons. The movement of an electron is simulated by changing its position using regular time increments dt . The displacement vector $\Delta\mathbf{x}$ is determined by

$$\Delta\mathbf{x} = |\mathbf{v}|dt.$$

The value of dt is chosen so that the mean free path L_{MPF} is much larger than the average magnitude of the coordinate change vector ($L_{\text{MPF}} > \langle \Delta x \rangle$). Only the electron-phonon interaction was taken into account. In the electron-phonon interaction, an electron can either receive

or give away energy, and its direction of motion changes randomly. The probability of scattering by a phonon at the next iteration was calculated using the formula [1]:

$$p_{\text{scat}}(E) = 1 - \exp\left(-\frac{\Delta x}{L_{\text{MPF}}}\right).$$

The last simulation stage is boundary collision: if the electron crosses the interface between the semiconductor and vacuum, then the conditions of energy and momentum conservation are checked. If the test is passed, it is assumed that the electron has been emitted into the vacuum. The simulation ends for this electron. The simulation also ends if the electron has lost too much energy due to electron-phonon interactions, namely, if its energy becomes less than the phonon energy. If the above conditions are not met, then the electron is elastically reflected from the surface into the semiconductor, and the transport simulation continues.

To calculate QE and intrinsic emittance, many independent simulations of the electron motion are performed at different initial positions and energies. The electrons do not interact with each other.

The QY is calculated using the expression:

$$J(\hbar\omega) = \frac{N_{\text{emission}}(\hbar\omega)}{N_{\text{el}}}.$$

Here, N_{emission} is the number of released electrons, and N_{el} is the number of electrons for which the simulation was performed.

The beam divergence θ_{div} of the emitted electrons, which characterizes the angular spread of the photoelectron beam, is calculated as:

$$\theta_{\text{div}} = \frac{\sqrt{\langle p_{\perp}^2 \rangle}}{mc},$$

where $\langle p_{\perp}^2 \rangle$ is the root mean square of the transverse momentum of the escaping photoelectrons, c is the speed of light, and m is the electron mass. Following the common practice in photocathode literature [1,4,5], we refer to this quantity θ_{div} as the intrinsic emittance normalized to the laser spot size (unit: mm · mrad/mm).

A. Surface plasmon polaritons

Works [4,5] have shown that SPPs enable a significant increase in QE. To excite plasmon resonance, a grating was applied to the photocathode, as shown in Fig. 2. This figure shows the cells in which the simulation was performed. Periodic boundary conditions were established along the OX and OY axes. The wave propagates along the OZ axis. The physics of SPPs has been discussed in detail in [5].

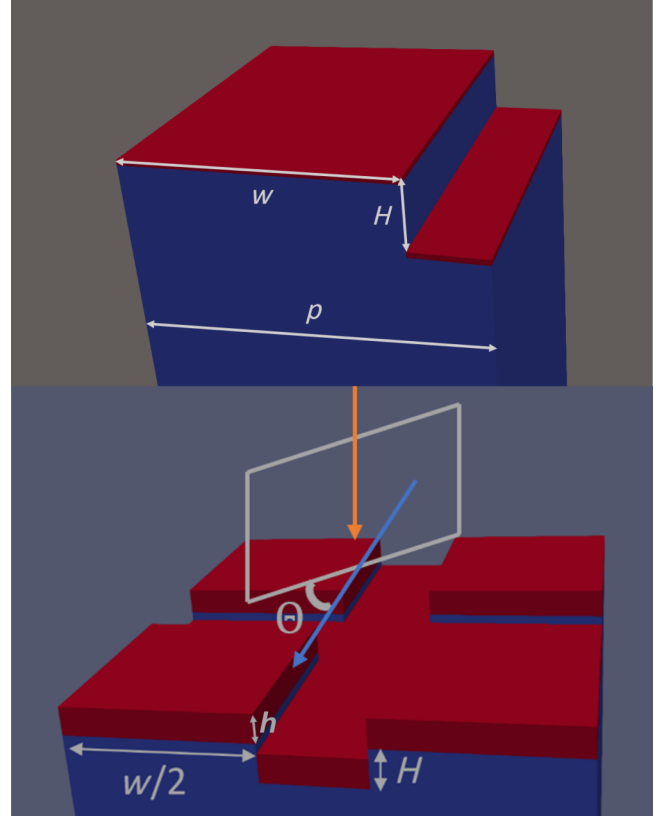


FIG. 2. Geometry of photocathodes: 1D and 2D gratings. The cathode layer is marked in red, h is the thickness of the cathode layer.

Within this chapter, we will provide only a brief description of the conditions for SPPs excitation.

The dispersion relation for plasmons allows one to derive the resonance condition from the optical parameters of the materials. This relation holds for the interface between a semiconductor and a metal with dielectric permittivities ϵ_1 with ϵ_2 , respectively:

$$\beta_{\text{spp}} = |\mathbf{k}| \sqrt{\frac{\epsilon_1 \epsilon_2}{\epsilon_1 + \epsilon_2}}, \quad (2)$$

where $|\mathbf{k}|$ is the wave vector module in vacuum and β_{spp} is the propagation constant of the SPPs. If the real part of the fraction's argument is greater than zero, plasmon resonance can occur.

If the wave vector $\mathbf{k}$ is directed normally to the photocathode surface, plasmonic modes are described by the following relation:

$$\beta_{\text{SPP}} = u \frac{2\pi}{p}. \quad (3)$$

Here, $u = (1, 2, 3, \dots)$ is an integer. From Eqs. (2) and (3), it is possible to obtain wavelengths at which plasmon resonance is expected to occur.

IV. RESULTS

We investigated three types of photocathode geometries: without SPPs (flat interface), with a 1D grating, and with a 2D grating. The process of optimizing geometric parameters to maximize QE at the wavelength of 2.32 eV (532 nm) is described. Lasers operating at this wavelength are commonly used in laboratory practice. For both 1D and 2D gratings, the dependence of the QE spectrum on the rotation angle of the polarization plane under normal light incidence is presented. A comparison with a photocathode without SPPs is performed. For all grating types, we examine the dependence of emittance on the wavelength.

A. Comparison with experimental data

As an initial step to verify the correctness of the computational model, we validated its results by comparing them with experimental data for a nonstructured semiconductor. The flat structure is described by a single geometric parameter h , the thickness of the semiconductor film. To the best of our knowledge, there is no experimental data on the QE of nanostructured semiconductor photocathodes.

The QE spectrum of a K_2CsSb photocathode at a temperature of 300 K is presented in [1]. The cathode consists of a thick molybdenum substrate and a 40-nm-thick layer of K_2CsSb semiconductor. The simulation was performed in the range from 1.8 to 2.4 eV. At these energies, the influence of electron-electron scattering for K_2CsSb is small, and our model remains valid.

Based on this distribution and Eq. (1), the initial conditions for the Monte Carlo transport simulation were defined. The parameters for the computational experiment, such as the density of states (DoS) of K_2CsSb [23] and the optical constants of molybdenum [24], were taken from the literature. A set of input parameters with references is provided in Table I; we used the number of electrons $N_{el} = 80\,000$.

The FDTD simulation was performed with a spatial step of $dx = 1$ nm. The semiconductor thickness corresponds to 40 spatial FDTD cells. With the chosen spatial step, a typical condition $\lambda/dx > 20$ is satisfied that ensures sufficient accuracy for the FDTD simulation. The

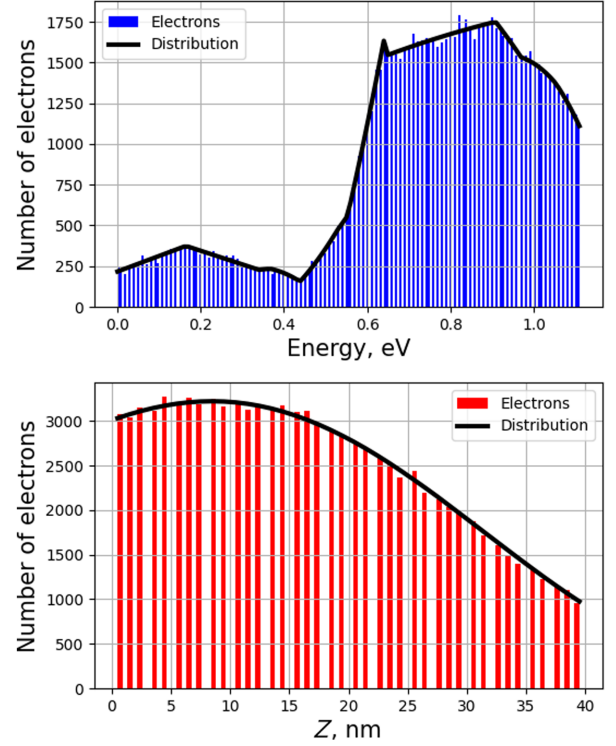


FIG. 3. Distribution of energy and position of the excited electron. The Z axis is oriented along the normal to the semiconductor surface. The origin corresponds to the semiconductor-vacuum interface. Energy is measured from the bottom of the conduction band.

calculated distribution of light absorption within the cathode was then used to determine the initial spatial distribution of the electrons.

The initial energies and coordinates of the electrons were randomly chosen based on the distributions determined by the absorbed light intensity and the DoS of K_2CsSb . The initial electron distribution is presented in Fig. 3. The energy corresponding to the lower edge of the conduction band was taken as zero.

In the transport simulation, the photocathode geometry was represented by two planes: the one defining the semiconductor-metal interface and the other the semiconductor-vacuum interface. The distance between the planes was 40 nm.

Comparison of the combined MC and FDTD simulation results with the experimental data is presented in Fig. 4. All parameters for K_2CsSb were set as in Ref. [1], except for the electron L_{MPF} . The need for adjustment arises from our use of a triangular emission barrier [20], more suitable for low-affinity semiconductors than a step-function model. With $L_{MPF} = 3$ nm, this model underestimates the QE (Fig. 4, red solid curve). Switching to a step-function barrier removes this discrepancy (Fig. 4, red dashed curve), aligning the result with Ref. [1]. To maintain the triangular barrier while matching the

TABLE I. Simulation parameters for K_2CsSb .

	Value	Unit	Source
L_{MPF}	5	nm	[13]
E_g	1.2	eV	[1]
E_a	0.5	eV	[1]
E_{ph}	0.027	eV	[1]
T	300	K	[1]
m_{eff}	0.117		
dt	0.1	fs	

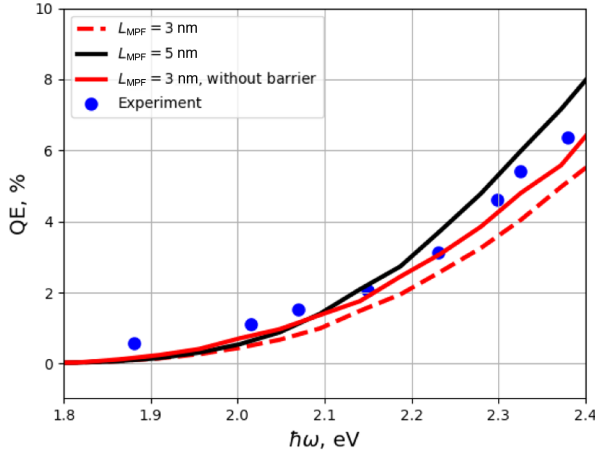


FIG. 4. K_2CsSb 40 nm film on molybdenum substrate. Black solid curve: simulation with $L_{\text{MPF}} = 5$ nm and a triangular emission barrier. Red solid curve: simulation with $L_{\text{MPF}} = 3$ nm and without the triangular barrier. Red dashed curve: simulation with $L_{\text{MPF}} = 3$ nm and with the triangular barrier. Blue points: experimental data from Ref. [1].

experiment, we adopted $L_{\text{MPF}} = 5$ nm [17] for all further simulations. We did not optimize but took the most suitable parameter from those used for modeling alkali semiconductors. Despite some quantitative discrepancies with the experiment, the QE dependence for a flat semiconductor is reproduced with sufficient accuracy for the following studies.

B. Grating design

The 1D and 2D grating structures are described by four geometric parameters: the period p , the height of the metallic step H , the width of the step w , and the thickness of the cathode layer h . The parameters of the investigated geometries are presented in Table II.

The cathode layer of the investigated photocathode consists of the semiconductor K_2CsSb . It is deposited on a thick copper substrate. K_2CsSb is a popular cathode material, and copper is used as a substrate [25]. We performed simulations for photocathodes with a cathode layer thickness of 8 nm. This thickness is the one at which quantum effects are still sufficiently small, while it provides minimal photocathode response time [5].

Due to their resonant nature, SPPs enable QE enhancement only within a relatively narrow wavelength range. This necessitates different grating geometric parameters

for efficient operation in different spectral ranges. We considered a 1D grating optimized for the wavelength of 532 nm (2.32 eV).

Photocathodes with 1D gratings are polarization-sensitive due to the lack of rotational symmetry by $\pi/2$. If the light polarization is directed along the groove (p -polarization), SPPs are not excited [5]. We propose a photocathode design with a 2D grating as shown in Fig. 2(b). This structure possesses symmetry under rotation by $\pi/2$, and consequently, its QE is independent of the polarization of the incident light.

The grating's geometric parameters were optimized to maximize the QE at the wavelength of 532 nm. This is the wavelength of lasers frequently used in laboratory practice. To achieve the highest photocathode QE, a full optimization of the structure's geometric parameters is required. This means exploring various photocathode geometries and performing FDTD simulations first, followed by Monte Carlo simulations for each. The most computationally intensive part is the transport calculation using the Monte Carlo method. In this work, we employ a simplified algorithm for finding the maximum QE at 532 nm. It involves using only the FDTD method to calculate the absorption coefficient. We anticipate that the highest QE will be achieved when the highest absorption coefficient is attained.

From [4], it is known that the grating period has the greatest influence on the wavelength at which plasmon resonance is observed. The same work also indicates that the parameter w moderately affects the peak's position and its depth/intensity. The height parameter H weakly affects the absorption peak position but significantly affects its magnitude. Based on this information, the parameter optimization was organized as follows. The value of the period p was selected using Eqs. (2) and (3). Then, the width w is optimized, followed by the height H . At each stage, we select the value of the variable parameter for which the photocathode absorption is maximal. The conditions for plasmon resonance excitation are identical for the 1D and 2D gratings. Therefore, after optimizing the 1D structure, the same parameters can be applied directly to the 2D grating.

C. 1D and 2D gratings

Substituting the optical constants of copper and K_2CsSb into Eqs. (2) and (3) yields the grating period $p \approx 500$ nm at which plasmon resonance is expected to occur. The results of optimizing the geometric parameters of the photocathode are presented in Fig. 5. At the first stage, the parameter w was varied. The highest cathode absorption was observed at $w = 404$ nm. Similarly, the value of $H = 100$ nm was obtained. The absorption spectrum of the cathode with the best absorption coefficient is shown in Fig. 6. Compared to the geometry without a grating, there is a 60% gain in absorption.

TABLE II. Geometric parameters of gratings.

	P	w	H	h
Without SPPs	...	...	...	8
1D grating	512	404	100	8
2D grating	512	404	100	8

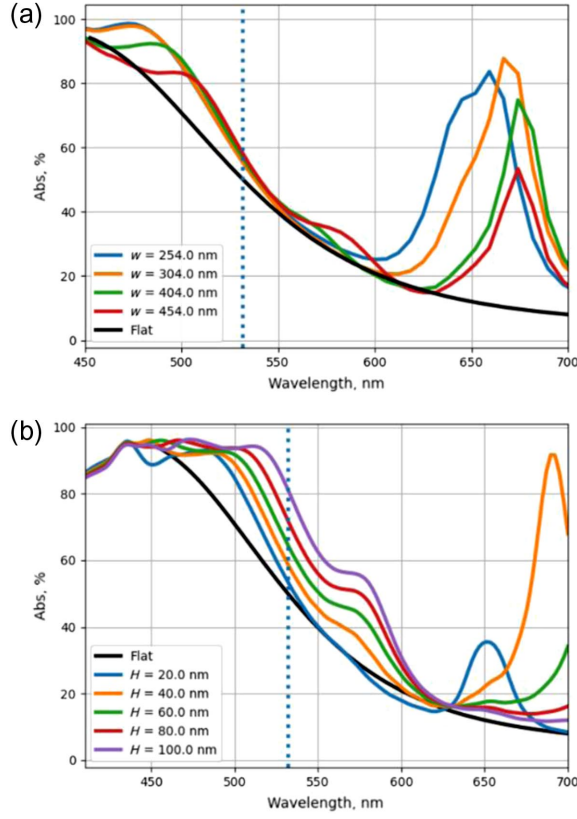


FIG. 5. Dependence of the absorption spectra of the photocathode on its geometric parameters. (a) Variation of w with a fixed period $p = 512$ nm and $H = 32$ nm; (b) variation of groove depth H with a fixed period $p = 512$ nm and width $w = 408$ nm. Semiconductor thickness is $h = 8$ nm.

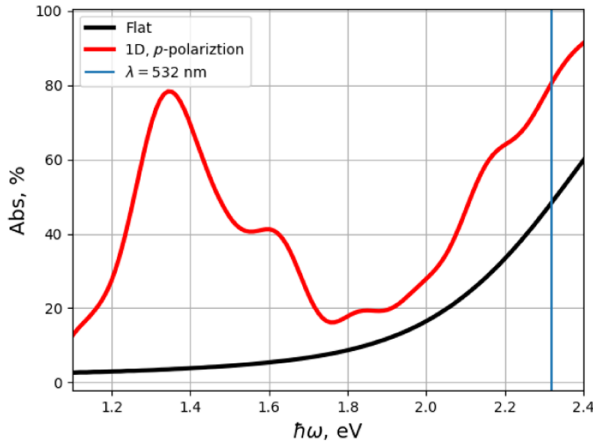


FIG. 6. Comparison of the absorption spectra of the photocathode with the 1D grating and a flat photocathode.

All optimization calculations were performed with the FDTD spatial step of 1 nm. Based on our results, the grating height parameter H has the greatest influence on the magnitude and width of the absorption peak and a slight influence on its position. By varying the structure

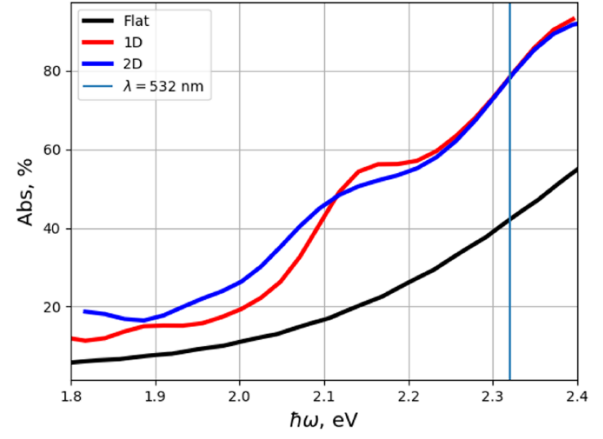


FIG. 7. Absorption spectra of photocathode without SPPs, 1D grating, and 2D grating.

period p and the step width w , it is possible to shift the absorption peak toward longer wavelengths. In general, our results are consistent with the conclusions of Ref. [4].

Comparing the absorption in Fig. 5 for photocathodes with and without SPPs, one can observe that SPPs produce two absorption peaks: in the infrared and visible parts of the spectrum. The most significant difference compared to a flat photocathode is observed in the long-wavelength region. However, with the photocathode parameters optimized for the wavelength of 532 nm, the second peak lies beyond the photoelectric threshold (red border). To shift it to shorter wavelengths, we modified the groove height H and the step width w .

We compared the photoemission characteristics of photocathodes with nanostructured and flat interfaces, both with a thickness of 8 nm. The absorption coefficients for 1D and 2D gratings are almost the same, see Fig. 7. The initial spatial distribution of electrons for a 1D photocathode is shown in Fig. 8(a), where regions of increased electron density are clearly distinguishable. These regions arise due to the local field enhancement induced by SPPs, which leads to a higher concentration of excited electrons. Figure 8(b) displays the coordinates of electron emission events on the photocathode surface. The locations of increased emission show a clear correlation with the areas of local field amplification.

The calculated QE spectra for the photocathode with a 1D grating are shown in Fig. 9. The parameters for K_2CsSb were set as specified in Table I. The QE increases across the entire spectral range. At the wavelength of 532 nm, the QE increases by 128%. SPPs do not have a strong influence on the cathode emittance (per unit of spot size) Fig. 10.

The following results were reported in [5]: the QE of the photocathode K_2CsSb with SPPs and thicknesses of 14, 16, 18, and 20 nm are approximately 17.33%, 19.40%, 17.15%, and 24.49%, respectively, at the wavelength 532 nm. There is a qualitative correspondence with our

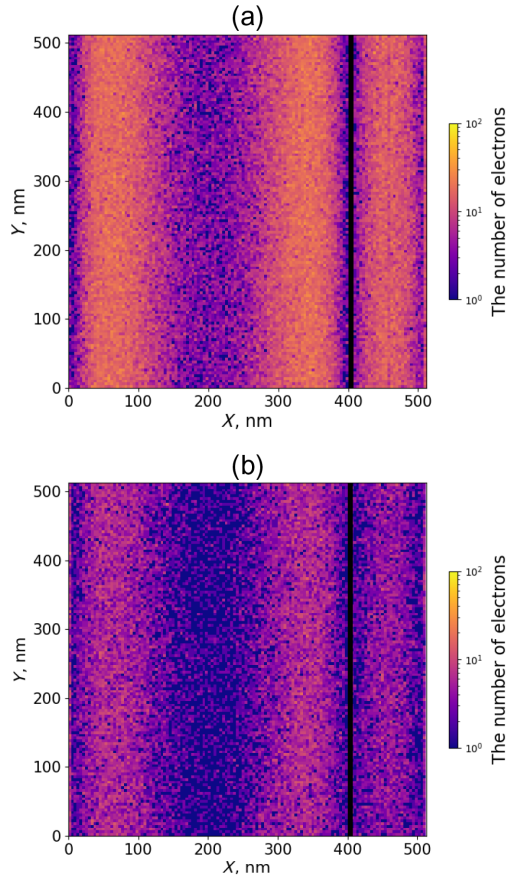


FIG. 8. Electron distribution for a 1D photocathode illuminated at a wavelength of 532 nm, p -polarization. The panels show a top view from the incident side. (a) Initial electron distribution at the start of the transport simulation. (b) Spatial coordinates of emission points where electrons escaped from the semiconductor into the vacuum. The color scale is identical for both panels. Black lines indicate the boundaries between different levels (steps) of the semiconductor layers along the OZ axis.

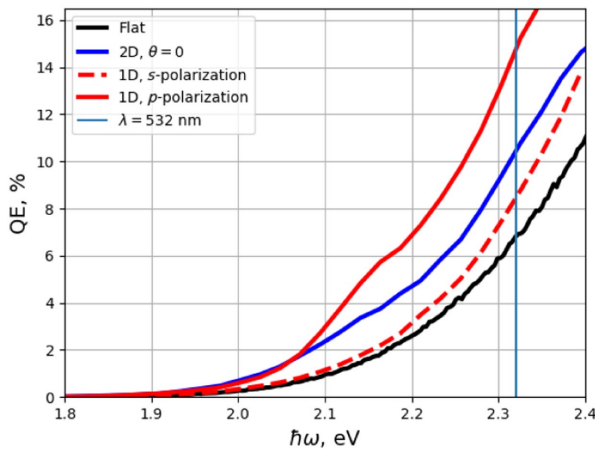


FIG. 9. The QE of 1D grating is polarization-dependent: p -polarization is directed parallel to the groove, and s -polarization is directed across the groove.

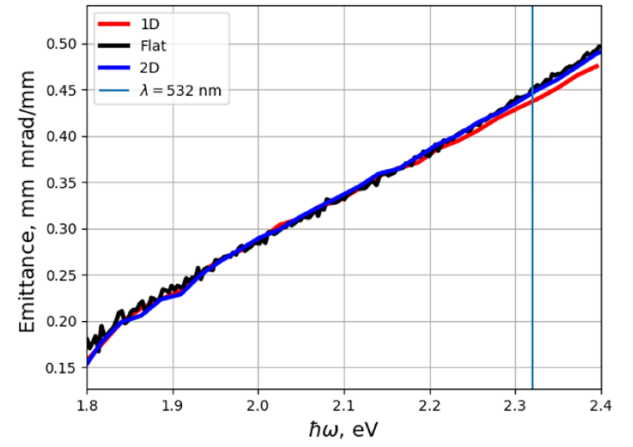


FIG. 10. Emittance normalized for the spot size of the laser for cathodes: cathode with 1D grating, 2D grating, and photocathode without SPPs.

results: we obtain the $QE = 15\%$ at the semiconductor thickness of 8 nm. The efficiency achieved in the present work is lower; this is due to a different substrate. Similar gratings were also studied in [4], where Cs_2Te was used as the cathode material. The SPPs have increased the efficiency by 60%.

We calculated the QE spectrum as a function of polarization: p -polarization corresponds to the case where the electric field vector is parallel to the grating grooves (the polarization plane normal is parallel to the grooves). If the electric field vector is perpendicular to the grooves, the wave has s -polarization. The QE for the p -polarized light increases significantly compared to the QE of a photocathode without SPPs. At the same time, for s -polarization, the QE of the photocathode with a grating does not substantially differ from the QE spectrum of a photocathode without a grating, see Fig. 9.

Generally, a structure with a 1D grating efficiently absorbs only one linear polarization, which limits its overall performance. To achieve high absorption efficiency for arbitrary polarization, we have proposed and studied a photocathode with a two-dimensional grating, the geometry of which is shown in Fig. 2(b).

As theoretically expected, the photocathode with a 2D grating exhibits polarization-independent performance. Three simulations were performed with different polarizations of the incident wave: for polarization rotation angles of $\theta = 0$ (electric field vector parallel to the grating trenches), $\theta = \pi/4$, and $\theta = \pi/8$. The simulation parameters were set as specified in Table I.

The initial electron distribution for the photocathode with a 2D grating is shown in Fig. 11(a). As in the case of the photocathode with a 1D grating, regions of increased electron density caused by SPPs are clearly distinguishable. Figure 11(b) shows the coordinates where electron emission was recorded.

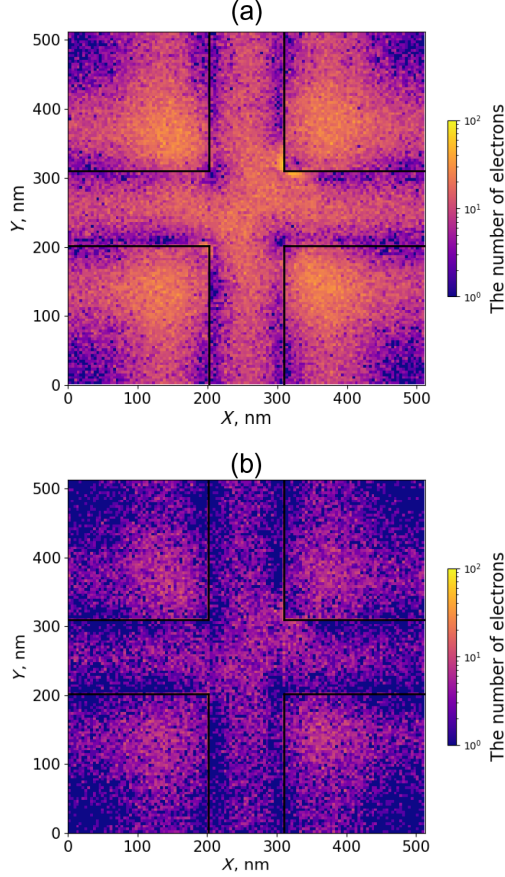


FIG. 11. Electron distribution for a 2D photocathode illuminated at a wavelength of 532 nm. The panels show a top view from the incident side. (a) Initial electron distribution at the start of the transport simulation. (b) Spatial coordinates of electrons escaped from the semiconductor into the vacuum. The color scale is identical for both panels. Black lines indicate the boundaries between different levels of the semiconductor layers along the OZ axis.

The simulation results confirm the assumption of polarization independence, see Fig. 12. However, the QE of the 2D grating is significantly lower at all polarizations than that of the 1D grating across almost the entire wavelength range (Fig. 9). The intrinsic emittance of a photocathode with a 2D grating is almost the same as that of a photocathode with a 1D grating, see Fig. 10. Applying a grating leads to a slight increase in emittance compared to a photocathode without SPPs.

V. DISCUSSION

The results for various grating types are summarized in Table III. We have calculated the QE enhancement as follows:

$$\text{QE enhancement} = 100\% \frac{\text{QE}(\hbar\omega) - \text{QE}_{\text{flat}}(\hbar\omega)}{\text{QE}_{\text{flat}}(\hbar\omega)},$$

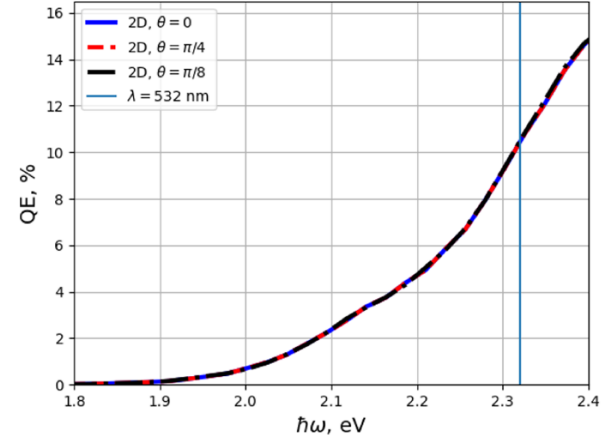


FIG. 12. The QE of the 2D grating with various incident wave polarizations. 2D grating is polarization-independent. The legend shows the polarization angle θ of the incident light. The differences between the spectra are almost indistinguishable: the average difference between the spectra does not exceed 0.01%.

where $\text{QE}_{\text{flat}}(\hbar\omega)$ is the QE of photocathode without SPPs. The QE of the 1D grating is 128% higher than that of the flat counterpart at the wavelength of 532 nm.

The influence of plasmon resonance is manifest not only in the increased absorption coefficient but also in the field localization. Let us call area 1 the region of the semiconductor at the top of the grating step and area 2 the region at the bottom of the groove. The areas are highlighted in Fig. 13. The dependence of the fraction of the field absorbed in the semiconductor $p_j(\hbar\omega) = \int_{V_j} d\rho_V(\hbar\omega)$ [see Eq. (1)] in different parts V_j of the cathode layer on the photon energy is shown in Fig. 14. At different wavelengths, the energy in the grating is distributed in different ways. At low energies, the main contribution to photoemission is made by area 1. As the photon energy increases, the contribution of area 2 increases, and that of area 1 decreases. At a photon energy of 1.2 eV, these contributions become equal.

TABLE III. Comparison of the key performance metrics of different photocathode designs: a flat surface (reference) and two types of nanoscale gratings (1D and 2D gratings). The compared metrics are the QE, the relative QE enhancement compared to the flat design, the operating energy range for peak performance, and whether the response is independent of light polarization.

	QE(%)	QE enhancement (%)	Polarization independence
Without SPPs (flat)	6.9($\lambda = 532$ nm)	...	Yes
1D grating	15.25($\lambda = 532$ nm)	128	No
2D grating	11.45($\lambda = 532$ nm)	54	Yes

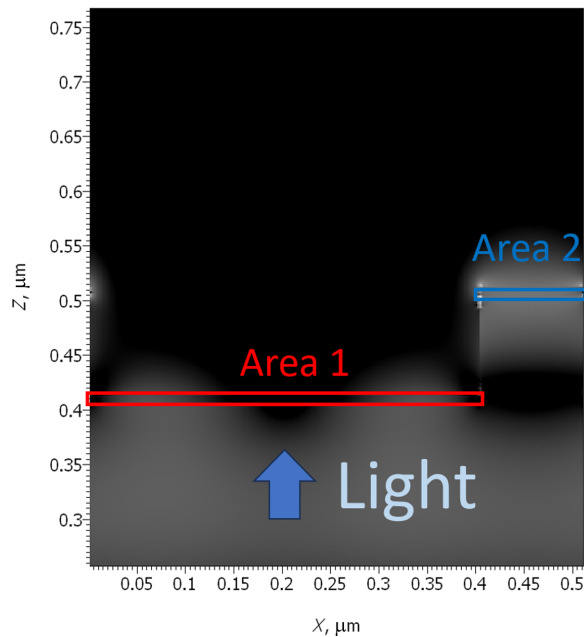


FIG. 13. Distribution of the electric field magnitude in a 1D grating. Various semiconductor regions are highlighted. Area 1 is the area at the top of the groove, and area 2 is at the depth. The wavelength is 533 nm.

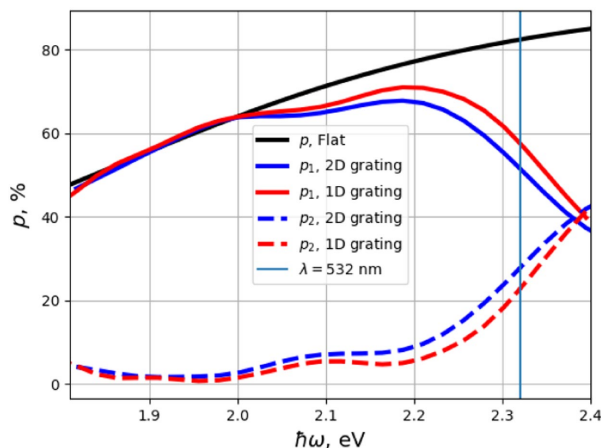


FIG. 14. Contributions of the fraction of the field absorbed in the cathode layer of photocathode without SPPs and different segments of photocathodes with 1D and 2D gratings: p_1 is the fraction of photons absorbed by the semiconductor on top of the “step,” and p_2 is the fraction of photons absorbed by the semiconductor deposited at the bottom of the groove. At the wavelength of 532 nm, most of the field is absorbed on top of the “step.”

The differences in QE between 1D and 2D structures can be attributed to the distinct localization of the field. In the case of the 1D, the primary contribution to QE comes from area 1, which is situated on top of the grating. As seen from Fig. 14, this is also true for the two-dimensional structure; however, the relative size of the analogous

region is smaller in this case. If we assume that the groove step makes the main contribution to quantum efficiency, then the quantum outputs for 2D and 1D should be correlated as relative areas of the regions. The relative size of the top surface for the 1D grating is w/p , but for the 2D grating, it is w^2/p^2 . Thus, the relative size of the 1D grating top surface is 25% larger than for the 2D grating. This explains the $\sim 25\%$ difference in QE between the 1D grating (QE = 15.25%) and the 2D grating (QE = 11.45%) at the wavelength of 532 nm.

VI. CONCLUSIONS

A multiphysics technique, extending the coupled FDTD—Monte Carlo approach, has been developed and validated for the three-dimensional simulation of the photoemission processes in nanopatterned photocathodes composed of K_2CsSb .

The developed technique made it possible to describe the effect of SPPs on the excitation, transport, and output of photoelectrons from the cathode for systems with a cathode layer thickness comparable to the free path of an electron and a 2D grating.

The parameters of semiconductor photocathodes with SPPs have been investigated, and their absorption coefficients optimized. It is shown that the QE of photocathodes with SPPs is significantly (by 128%) higher than that of photocathodes without SPPs. It is established that the gratings do not impair the intrinsic emittance.

The dependence of the QE of photocathodes with 1D and 2D gratings on the polarization of illumination was studied. Calculations have shown that the main advantage of the developed 2D gratings is their polarization independence.

The developed technique can also be applied to the modeling of photocathodes based on Cs_3Sb , Cs_2Te , $CsNa_2KSb$, Cs_2KSb , and other alkali semiconductors.

While the modeling results are promising, the experimental implementation of the K_2CsSb structure on a copper substrate requires careful consideration. Early studies reported significant interaction between the deposited material and the copper surface, which could compromise the photocathode performance [25,26]. However, more recent work has shown that with appropriately optimized growth procedures, high-quality K_2CsSb photocathodes can be successfully fabricated on copper substrates [27]. For the ultrathin plasmonic geometry considered in this work, the interface may be particularly sensitive, and therefore, the application of interface passivation techniques could be beneficial to ensure stable and reproducible performance.

DATA AVAILABILITY

The data that support the findings of this article are openly available, embargo periods may apply [28].

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