Multiphysics Modeling of Plasmonic Photoconductive Devices using Discontinuous Galerkin Methods

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Abstract

Plasmonic nanostructures can significantly improve the performance of photoconductive devices (PCDs). In the mean time, they introduce intricate structures and complex scattering, which lead new challenges to simulations. In this work, a multiphysics framework based on discontinuous Galerkin (DG) methods is proposed to model the nonlinearly-coupled multiphysics processes in plasmonic PCDs. Without optical pumping, the nonequilibrium steady-state of the device, described by a coupled Poisson/drift-diffusion (DD) system, is solved with the Gummel iteration method. With pumping, the wave scattering, carrier dynamics and their nonlinear interactions are modeled by an explicit time domain solver solving the coupled system of Maxwell/time-dependent DD equations. The DD equations and Poisson equation are discretized with the local DG method and Maxwell equations are discretized with the nodal DG method. The DG-based multiphysics framework provides favorable discretization flexibilities for modeling the multiscale features in plasmonic PCDs. The proposed framework is demonstrated with simulations of a conventional PCD and a plasmonic PCD.

Index Terms

Discontinuous Galerkin method, drift-diffusion equations, Maxwell equations, multiphysics modeling, optoelectronic devices, Poisson equation, semiconductor device simulation.

I. INTRODUCTION

In recent years, terahertz (THz) devices have become indispensable components of electromagnetic (EM) systems in applications ranging from wireless communication to non-destructive testing. The main obstacle in the way of widespread industrial use of THz technologies is the difficulty of the implementing compact, efficient, frequency-stable and tunable THz source generators capable of operating at room temperatures. Plasmonic photoconductive devices (PCDs) have become one of the most promising candidates for THz source generation because of their dramatically increased optical-to-THz conversion efficiency and polarization insensitivity [1]–[3]. While the experimental research on plasmonic PCDs has made rather significant progress, rigorous numerical modeling of this type of devices is still challenging.

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Challenges in the simulation of PCDs reside in the multiphysics nature of the involved physical process. PCDs are based on photoconductive semiconductor devices, which generate carriers under optical pumping and produce THz currents under the driving force of an applied bias voltage [4], [5]. Physically, a PCD has two operation stages: (1) a steady-state corresponding to the non-equilibrium state of the semiconductor device under a bias voltage; (2) a transient-stage describing the dynamic process after a pumping laser impinges upon the device. The steady-state involves the interaction between electric potential and carrier dynamics, which is usually described by a coupled system of Poisson equation and drift-diffusion (DD) equations. In the transient-stage, several processes happen simultaneously: EM wave scattering, carrier generation and recombination, carrier drift driven by electric fields, and carrier diffusion. This stage can be described by a coupled system of Maxwell equations and time-dependent DD equations. Due to the strong nonlinear coupling between carriers and EM waves, especially the exponential growth of carrier densities upon the absorption of light, accurate modeling of this process calls for a time domain multiphysics solver.

Moreover, due to the involvement of different physics, characteristic scales in this device also differ by several orders of magnitude. Length scales range from $\sim 10\text{nm}$ (Debye screening length) to $\sim 1\mu\text{m}$ (the device geometry features). Additionally, the plasmonic nanostructures and the localized plasmonic modes make the length scale even more complicated. Time scales are signified by carrier dynamics (including the advection and diffusion motions), the EM wave propagation, and the response time between their coupling. Those scales typically differ by $2 \sim 3$ orders of magnitude. The multiscale nature requires highly flexible discretization schemes. Furthermore, the long physical time, regarding to the ratio between the THz wave period and the optical wave period, requires high order accuracy in time integration.

Several numerical approaches have been proposed for PCDs simulations. For conventional PCDs, the finite difference time domain (FDTD) method has been extensively used [6]–[10]. In this approach, an analytic carrier generation rate is used to model the optical pumping. The carrier dynamics is modeled with time-dependent DD equations and Maxwell equations are used to model the THz radiation. All equations are solved with finite difference methods. For conventional PCDs, this approach has been shown to agree with experiments very well [7]–[9]. However, for plasmonic PCDs, this approach turns out to be inadequate. In plasmonic PCDs, a crucial design is the nanostructure, which can produce enhanced local EM fields and hence enhance the carrier generation. The nanostructure leads strong scattering of the pumping EM wave, making the previously used analytic generation rate invalid. Meanwhile, the plasmonic structures and the plasmonic mode patterns are rather complicated, which require prohibitively dense meshes if using orthogonal FDTD grids. Several other methods are also reported, e.g., in [11], [12] the frequency domain optical field solution is used to estimate the time-modulated carrier generation and the transient-stage is modeled with a coupled Poisson-DD solver, in [13] an equivalent circuit model is used to estimate the optical-to-THz conversion efficiency, in [14] the semiconductor device is treated as a one dimensional port model and the EM radiation is solved with the discontinuous Galerkin finite element time domain method. Although those approaches are efficient for the conventional PCDs, the adopted approximations make them inadequate for plasmonic PCDs due to the complicated scattering of the pumping EM wave.

To model plasmonic PCDs, recent works utilize the finite element method (FEM) [15], [16]. Taking advantages
of the unstructured meshes in FEM, this approach can easily solve the complex EM field in the plasmonic
nanostructures. The carrier generation is calculated from the EM field and used in time domain carrier dynamics
simulations. However, because of using frequency domain FEM, the space-distribution of the carrier generation is
considered as time-invariant and the time-dependency is approximated by an analytic pulse shape. This means the
nonlinear coupling between EM waves and carriers is not fully considered in this approach. In practice, the EM
scattering, the carrier generation, and carrier movements happen simultaneously. Due to the scattering of the pumping
EM wave, the carrier generation rate is space-time dependent. The generated nonuniform carriers in turn lead to
scattering of the optical EM wave, which will again change the carrier generation. Since carrier densities increase
exponentially as the pumping wave energy is absorbed, the whole process is strongly nonlinear. Furthermore, the
space-charge screening effect, i.e., the separation of electrons and holes induces polarization that cancels the electric
field, which depends on time-varying carrier distributions, is not captured in the FEM-based approach. This effect
is important for understanding the high-power saturation effect in PCDs and has been extensively studied [4], [17],
[18].

In this work, we propose a multiphysics framework for modeling plasmonic PCDs using the discontinuous
Galerkin (DG) methods [19]–[21]. The device is modeled in two stages as the physical operation stages described
above. The steady-state is solved by a nonlinear solver solving a coupled system of Poisson equation and bipolar
DD equations. The transient-stage is modeled by solving time-dependent Maxwell equations and DD equations
simultaneously, with the nonlinear couplings between carriers and EM waves being fully taken into account. The two
solvers are connected by separating static and time-dependent variables. All equations are solved with DG methods.
DG methods provide high flexibility in meshing (as FEM does) and allow explicit time integration (like FDTD).
By using high-order basis functions and high-order time integration schemes, they can easily achieve high-order
accuracy. In addition, DG methods provide advanced features such as non-conformal meshes, adaptive hp-refinement,
and local time stepping. When using explicit time integration, they also show high parallel efficiencies, making them
efficient on clusters. Those properties make DG methods promising for multiphysics and multiscale simulations [22],
[23]. In the context of plasmonic PCDs, plasmonic structures and plasmonic modes can be modeled easily using
unstructured meshes and the nonlinear couplings in the optical-to-THz conversion process can be captured naturally
with explicit time integration. The flexible discretization also allows using different meshes and time step sizes for
different equations, which can alleviate the computational effort a lot when dealing with the multiscale features.

This paper is organized as follows. Section II describes the physical processes involved in plasmonic PCDs. Two
nonlinearly coupled systems are introduced to describe the steady-state and the transient-stage. Section III presents
the numerical approach dealing with the nonlinear couplings and the DG discretization for each equation. Two
examples are presented in Section IV, where a conventional PCD is modeled and compared with references and a
plasmonic PCD simulation is presented to demonstrate the capability of the proposed framework. Finally, Section
V concludes this paper with some remarks on applications of the multiphysics framework.
II. FORMULATION

A. Physical Model

PCDs are based on photoconductive semiconductors, of which the low temperature grown gallium arsenide (LT-GaAs) is the most popular one. LT-GaAs has electron trapping time less than 1 picosecond (ps) and a direct optical band gap of 1.42eV. They can absorb optical wave energy and generate pulsed photocarriers with pulse width $< 1$ ps, providing THz components. A typical PCD device has two electrodes deposited on the photoconductive semiconductor substrate. The electrodes are biased by an external voltage, which can drive the photocarriers into the electrodes. In the meantime, the electrodes act as parts of a radiating THz antenna. In conventional PCDs, the optical-to-THz conversion efficiency is limited by the amount of the absorbed optical energy, which is usually small due to the high refractive index of LT-GaAs.

Plasmonic PCDs utilize metallic nanostructures to increase the optical-to-THz conversion efficiency. The nanostructures are designed to introduce plasmonic resonances at the operating optical frequency, which can greatly enhance the local EM fields and increase the light absorption. Aside from introducing plasmonic resonances, the nanostructures, which are either placed in-between the gap of the electrodes or etched into the electrodes, also change the electric potential distribution and the distance between photocarriers and electrodes. The latter effects also significantly influence the photocurrent [24]. Thus, the design of the nanostructures is not only to optimize the plasmonic EM modes, but to optimize the overall photocurrent response. Another factor of the device design is the impedance matching between the semiconductor layer and the THz antenna. However, this factor seems not so critical as the photocurrent generation, as is reported in several experimental reports [1], [15], where the output THz radiation power is observed to be proportional to the photocurrent. Thus, in this work, we focus on modeling the photocurrent generation and the THz radiation is not discussed.

Physical description of this device includes carrier dynamics and electrodynamics (including the bias electric field and EM waves corresponding to the pumping light and the THz radiation). While Maxwell equations are used to describe electrodynamics, various models exist for describing carrier transport in semiconductor devices, ranging from semi-classical to quantum approaches. For PCDs, the semi-classical DD model is widely used [8], [25], [26] since the device size ($\sim 10\mu$m) is far larger than the mean free path of the carriers ($\sim 0.01\mu$m). Regarding the difference of parameters for electrons and holes, and the space-charge screening effect, the bipolar DD equations are considered. Thus, the coupled system of electrodynamics and carrier dynamics is described by the following coupled equations

\begin{align}
\mu(r)\partial_t H(r, t) &= -\nabla \times E(r, t) \\
\varepsilon(r)\partial_t E(r, t) &= \nabla \times H(r, t) - [J_e(r, t) + J_h(r, t)] \\
q\partial_t n_c(r, t) &= \pm \nabla \cdot J_e(r, t) - q[R(n_e, n_h) - G(E, H)] \\
J_e(r, t) &= q\mu_e(E)E(r, t)n_e(r, t) \pm qd_e(E)\nabla n_e(r, t)
\end{align}

where $r$ represents the location vector, the subscript $c \in \{e, h\}$ represents the carrier type and hereafter the upper and lower signs should be selected for electron ($c = e$) and hole ($c = h$), respectively, $E(r, t)$ and $H(r, t)$ are the
total electric and magnetic field intensities, $\varepsilon(r)$ and $\mu(r)$ are the dielectric permittivity and permeability, $n_e(r, t)$ and $n_h(r, t)$ are the total electron and hole densities, $J_e(r, t)$ and $J_h(r, t)$ are the total electron and hole current densities, $R(n_e, n_h)$ and $G(E, H)$ are the recombination rate and the generation rate, respectively. We note that Gauss law is implicitly included in (1)-(3). In (4), $\mu_e(E)$ and $\mu_h(E)$ are the field-dependent electron and hole mobilities, $d_e(E) = V_T \mu_e(E)$ and $d_h(E) = V_T \mu_h(E)$ are the electron and hole diffusion coefficients, respectively.

In PCDs, a biased voltage is added on the electrodes throughout operation process. Before turning on the optical pump, the device is under a non-equilibrium steady-state [27]. When the pump pulse enters the device, the EM wave energy is absorbed by the semiconductor and photocarriers are generated. Since the photocarrier density is several orders of magnitude smaller than the doping concentration, the biased steady-state is only weakly perturbed by the pumping. Thus, the total fields, the total carrier densities, and the total current densities can be separated into steady-state DC components and transient components as $E(r, t) = E^s(r) + E^t(r, t)$, $H(r, t) = H^s(r) + H^t(r, t)$, $n_e(r, t) = n_e^s(r) + n_e^t(r, t)$, $J_e(r, t) = J_e^s(r) + J_e^t(r, t)$, respectively. Here, the superscript “s” and “t” stand for steady-state and transient (time-dependent) variables, respectively.

Similarly, the total recombination rate in (3) is divided as $R(n_e, n_h) = R^s(n_e^s, n_h^s) + R^t(n_e^t, n_h^t)$, where $R^s(n_e^s, n_h^s)$ describes the recombination rate of steady-state carriers and $R^t(n_e^t, n_h^t)$ describes the recombination rate of photocarriers. In this work, we consider the two most common processes, namely the trap assisted recombination described by the Shockley-Read-Hall (SRH) model [26], [27]. The generation rate is defined as

$$G(E', H') = \frac{\eta \alpha \lambda I(E', H')}{hc}$$  \(5\)

where $\lambda$ is the pumping wavelength, $\alpha$ is the photon absorption coefficient, $\eta$ is the quantum yield, $h$ is the Planck constant, $c$ is the light speed, and $I(E', H')$ is the energy flux density of the optical wave

$$I(E', H') = \frac{1}{T} \int_0^T |E'(r, t) \times H'(r, t)| \, dt$$  \(6\)

which only depends on the time-dependent EM fields of the optical wave. Here, using the energy flux density allows us to model the carrier generation in the complicated space-time varying EM fields (resulted from the scattering from the plasmonic nanostructures and the nonuniformly distributed carriers). It is justified by the fact that the optical pump dominates the energy flux density and the contribution from THz frequency components is ignorable in the semiconductor substrate. If monochromatic wave is considered, the energy flux density returns to the optical intensity, which is widely used in analytical estimations [8], [12], [15], [16], [25].

In general, when using the DD model to simulate nonequilibrium state of semiconductor devices, one should consider field-dependency and velocity-saturation in the mobility model. Because mobility influences the carrier drift velocity, it is important to consider appropriate models for the photocurrent modeling. Here, we use the parallel-field dependent mobility model reported in [8]. Since $E^s(r)$ is two orders of magnitude stronger than $E^t(r, t)$, $E^t(r, t)$ is ignored in the field-dependent mobility model.
Regarding to the fact that the steady-state components satisfy the coupled system of Poisson and DD equations

\[
\nabla \cdot (\varepsilon(r)E^s(r)) = q(C + n_h^s(r) - n_e^s(r)) \tag{7}
\]

\[
\nabla \cdot J^s_e(r) = \pm qR^s(n_e^s, n_h^s) \tag{8}
\]

\[
J_e^s(r) = q\mu_e(E^s(r))E^s(r)n_e^s(r) \pm qd_e(E^s)\nabla n_e^s(r) \tag{9}
\]

the static components can be eliminated from the time derivative and the right hand side terms of (2)-(4), resulting the reduced Maxwell-DD system

\[
\mu \partial_t H^t(r, t) = -\nabla \times E^t(r, t) \tag{10}
\]

\[
\varepsilon \partial_t E^t(r, t) = \nabla \times H^t(r, t) - [J^t_e(r, t) + J^t_h(r, t)] \tag{11}
\]

\[
q \partial_t n_e^t(r, t) = \pm \nabla \cdot J^t_e(r, t) - q[R^t(n_e^t, n_h^t) - G(E^t, H^t)] \tag{12}
\]

\[
J^t_e(r, t) = q\mu_e(E^s)((E^s(r) + E^t(r, t))n_e^t(r, t)
+ E^t(r, t)n_e^t(r, t)) \pm qd_e\nabla n_e^t(r, t). \tag{13}
\]

Here we should note that the same separation of variables has been done in [14].

Equations (11)-(13) is a strongly-nonlinear system. In (12), \(G(E^t, H^t)\) leads to exponential increasing of carrier densities. In (13), carriers are driven by both \(E^t(r, t)\) and \(E^s(r)\). The carrier motion produces free current densities \(J^t_e(r, t)\) and \(J^t_h(r, t)\), which results in EM wave scattering. This is described by the current term in (11). The EM wave scattering, in turn, changes \(G(E^t, H^t)\). \(R^t(r, t)\) is also a nonlinear function, which becomes significant when carrier densities are high, balancing the carrier generation.

B. The Multi-physics DG Solver

A complete simulator for PCD comprises a steady-state solver solving the Poisson-DD system (7)-(9) and a transient solver solving the Maxwell-DD system (10)-(13). The steady-state solutions are used as input parameters of the transient solver. The steady-state is solved by a nonlinear solver making use of the Gummel iteration method. For details, we refer the reader to [27]. Here, we focus on the transient solver.

1) Nonlinear Coupling: To solve the time-dependent Maxwell-DD system, we use an explicit time integration approach. Regarding the difference of time scales in EM wave propagation and carrier dynamics, Maxwell and the DD equations are updated separately as two subsystems. Such that we can use different time step sizes in the two subsystems. In PCDs, carriers response much slower than the variation of EM fields. Hence we can update the DD equations with a larger time step size without sacrificing accuracy. The nonlinear couplings between two subsystems are handled by alternately feeding updated solutions into each other.

The updating procedure is shown in Fig. 1, where the time step size for the DD equations is assumed to be twice the step size for Maxwell equations for illustration. Let us suppose the two systems are updated separately with certain time integration schemes (to be discussed in the next subsection) and denote the time steps of the Maxwell and DD systems as \(T\) and \(T'\), respectively.
Assuming that both subsystems are synchronized at step $T$ and $T'$ (with the same physical time), first, $E^{T,T}$ and $H^{T,T}$ are used to calculate the generation rate $G^T$ using (5). $E^{T,T}$ and $G^T$ are used to update the DD equations from step $(T'-1)$ to $T'$ using (12). Then, the new carriers densities $n_{e,h}^{T'}$ are used to calculate the current densities $J_{e,h}^{T'}$ and $J_{e,h}^{T'+1}$, which are used in (11) to update Maxwell equations at steps $T$ and $(T+1)$, respectively. The physical time of two subsystems matches again at step $(T+2)$ and $(T'+1)$. One can again update DD equations to step $(T'+1)$ with the EM fields and generation rate at time step $(T+2)$.

2) Discretization: Both the time-dependent DD equations (12)-(13) and Maxwell equations (10)-(11) are solved with DG methods in time-domain. We start with the time-dependent DD equations (12)-(13). Since the electron and hole DD equations only differ in the sign in front of the drift term and the values of physical parameters, we only discuss the electron DD equation and, to simplify the notation, we drop the subscript “e” (denoting electron) and the superscript “t” (denoting transient) when there is no confusion. Furthermore, as the three drift terms in (13) are treated in the same way, for brevity, in the following formulation we only discuss one drift term and denote it as $v(r,t)n(r,t)$. The electron DD model (12)-(13) can be written as the following initial-boundary value problem (IBVP)

$$\frac{\partial}{\partial t} n(r,t) = \nabla \cdot \left[ d(r)q(r,t) \right] + \nabla \cdot [v(r,t)n(r,t)] - R(r,t), \quad r \in \Omega$$

(14)

$$q(r,t) = \nabla n(r,t), \quad r \in \Omega$$

(15)

$$n(r,t) = f_D(r), \quad r \in \partial \Omega_D$$

(16)

$$\hat{n}(r) \cdot [d(r)q(r,t) + v(r,t)n(r,t)] = f_R(r), \quad r \in \partial \Omega_R$$

(17)

where $q(r,t)$ is an auxiliary variable introduced to reduce the order of the spatial derivative in the diffusion term, $R(r,t) \equiv R'(n_e^s,n_h^s) - G(E^t,H^t)$, $\partial \Omega_D$ and $\partial \Omega_R$ represent the surfaces where Dirichlet and Robin boundary conditions are enforced, $\hat{n}(r)$ denotes the outward normal vector of the surface, and $f_D$ and $f_R$ are the coefficients associated with these boundary conditions, respectively. For the problems considered in this work, $\partial \Omega_D$ is set on electrode/semiconductor interfaces and $f_D$ is set as $n_e^s = 0$ (note that $n_e^s = (C + \sqrt{C^2 + 4n_i^2})/2$ and $n_h^s = n_i^2/n_e^s$ are imposed on the steady-state components based on local charge neutrality [27], [28]). The homogeneous Robin boundary condition $f_R = 0$ is used on semiconductor/insulator interfaces, indicating no carrier spills out those
interfaces [28].

To facilitate the numerical solution of the IBVP described by (14)-(17), \( \Omega \) is discretized into \( K \) non-overlapping tetrahedrons. The volumetric support of each of these elements is represented by \( \Omega_k, k = 1, \ldots, K \). Let \( \partial \Omega_k \) denote the element surface of \( \Omega_k \) and \( \hat{n}(r) \) denote the outward unit vector normal to \( \partial \Omega_k \). Testing (14) and (15) with Lagrange polynomials [19], \( \ell_i(r), i = 1, \ldots, N_p \), on element \( k \) and applying the divergence theorem yield the weak form

\[
\int_{\Omega_k} \partial_t n_k(r,t) \ell_i(r) dV = - \int_{\Omega_k} R(r,t) \ell_i(r) dV \\
- \int_{\Omega_k} d(r) q_k(r,t) \cdot \nabla \ell_i(r) dV \\
+ \oint_{\partial \Omega_k} \hat{n}(r) \cdot \{ d(r) q_k(r,t) \}^* \ell_i(r) dS \\
- \int_{\Omega_k} v(r,t) n_k(r,t) \cdot \nabla \ell_i(r) dV \\
+ \oint_{\partial \Omega_k} \hat{n}(r) \cdot \{ v(r,t) n_k(r,t) \}^* \ell_i(r) dS
\]

(18)

\[
\int_{\Omega_k} q_k^*(r,t) \ell_i(r) dV = - \int_{\Omega_k} n_k(r,t) \frac{\partial}{\partial \nu} \ell_i(r) dV \\
+ \oint_{\partial \Omega_k} \hat{n}_\nu(r) n_k^*(r,t) \ell_i(r) dS
\]

(19)

Here, \( N_p = (p+1)(p+2)(p+3)/6 \) is the number of interpolating nodes, \( p \) is the order of the Lagrange polynomials and \( \nu \in \{x,y,z\} \) is used for identifying the components of the vectors in the Cartesian coordinate system. We note that \( n_k(r) \) and \( q_k(r) \) are used to denote the local solutions on element \( k \) and the global solutions on \( \Omega \) are the direct sum of the local solutions.

\( n^*, (dq)^*, \) and \( (vn)^* \) are numerical fluxes “connecting” element \( k \) to its neighboring elements. Here, the variables are defined on the interface between elements and the explicit dependencies on \( r \) and \( t \) are dropped for simplicity of notation. For the diffusion term, the LDG alternate flux [29] is used for the primary variable \( n^* \) and the auxiliary variable \( (dq)^* \). For the drift term, the local Lax-Friedrichs flux [19] is used for \( (vn)^* \). In the interior of \( \Omega \), they are defined as

\[
n^* = \{n\} + 0.5 \hat{\beta} \cdot \hat{n} \|n\|
\]

\[
(dq)^* = \{dq\} - 0.5 \hat{\beta} (\hat{n} \cdot [dq])
\]

\[
(vn)^* = \{vn\} + \alpha \hat{n}(n^- - n^+).
\]

where average and “jump” operators are defined as \( \{ \circ \} = 0.5(\circ^- + \circ^+) \) and \( \| \circ \| = \circ^- - \circ^+ \), respectively, with \( \circ \) could be a scalar or a vector variable. Superscripts “-” and “+” refer to variables defined in element \( k \) and in its neighboring element, respectively. The vector \( \hat{\beta} \) determines the upwind direction of \( \varphi \) and \( (\varepsilon E) \). In LDG, it is essential to choose opposite directions for \( \varphi \) and \( (\varepsilon E) \), while the precise direction of each variable is not important [19], [20], [29]. In this work, we choose \( \hat{\beta} \) the same as \( \hat{n} \) on each element surface. The local Lax-Friedrichs, with \( \alpha = \max(|\hat{n} \cdot \mathbf{v}^-|, |\hat{n} \cdot \mathbf{v}^+|)/2 \), mimics the information propagation path of the directional
and \( \partial \Omega_D \), the numerical fluxes are chosen as \( n^* = f_D, (dq)^* = (dq)^- \) and \( (vn)^* = vf_D \). On \( \partial \Omega_R \), \( n^* = n^- \) and \( (dq)^* + (vn)^* = f_R \). We note that \( (dq)^* \) and \( (vn)^* \) are not assigned independently on \( \partial \Omega_R \).

Expanding \( n_k(\mathbf{r}, t) \) and \( q_k^*(\mathbf{r}, t) \) with Lagrange polynomials \( \ell_i(\mathbf{r}) \) [19]

\[
n_k(\mathbf{r}, t) \approx \sum_{i=1}^{N_p} n_i(\mathbf{r}, t) \ell_i(\mathbf{r}) = \sum_{i=1}^{N_p} n^i_k(t) \ell_i(\mathbf{r})
\]

(20)

\[
q_k^*(\mathbf{r}, t) \approx \sum_{i=1}^{N_p} q^i_k(\mathbf{r}, t) \ell_i(\mathbf{r}) = \sum_{i=1}^{N_p} q^i_k(t) \ell_i(\mathbf{r})
\]

(21)

where \( \mathbf{r}_i, \ i = 1, \ldots , N_p, \) denote the location of interpolating nodes, \( n^i_k(t) \) and \( q^i_k(t), \nu \in \{x, y, z\}, \ k = 1, \ldots , K, \) are the unknown coefficients to be solved for. Substituting (20) and (21) into (18) and (19), we obtain the semi-discretized form

\[
\begin{cases}
M_k \partial_t \hat{N}_k = \bar{C}_k \hat{N}_k + \bar{C}_{kk'} \hat{N}_{k'} + \\
\bar{D}_k \bar{d} \bar{Q}_k + \bar{D}_{kk'} \bar{d} \bar{Q}_{k'} - \bar{B}^n_k \\
\bar{M}^q_k \bar{Q}_k = \bar{G}_k \hat{N}_k + \bar{G}_{kk'} \hat{N}_{k'} + \bar{B}^q_k
\end{cases}
\]

(22)

where the unknown vectors are defined as \( \hat{N}_k = [n^1_k(t), \ldots , n^N_k(t)]^T \) and \( \bar{Q}_k = [Q^x_k, Q^y_k, Q^z_k]^T \), with \( Q^x_k = [q^\nu_k(t), \ldots , q^{N\nu}_k(t)] \), \( \nu \in \{x, y, z\} \).

In (22), \( M_k \) and \( M^q_k \) are mass matrices. \( M^q_k \) is a 3\( \times \)3 block diagonal matrix with each block the same as \( M_k \). \( M_k \) is defined as

\[
M_k(i, j) = \int_{\Omega_k} \ell_i(\mathbf{r}) \ell_j(\mathbf{r}) dV, \quad i, j = 1, \ldots , N_p.
\]

\( \bar{d} \) is a diagonal matrix with diagonal entries \( (d_1, \ldots , d_K) \), where \( d_k = (d^x_k, d^y_k, d^z_k), d^\nu_k(i) = d_k(\mathbf{r}_i), \ k = 1, \ldots , K, \ \nu \in \{x, y, z\}, \ i = 1, \ldots , N_p \). We note that \( d(\mathbf{r}) \) is assumed isotropic and constant in each element.

\( \bar{G}_k \) and \( \bar{G}_{kk'} \) are matrices corresponding to gradient operator and \( \bar{D}_k \) and \( \bar{D}_{kk'} \) are matrices corresponding to the divergence operator, respectively. Using the LDG flux, one finds \( \bar{D}_k = -\bar{G}^T_k \) and \( \bar{D}_{kk'} = -\bar{G}^T_{kk'} \). \( \bar{G}_k \) is a 3\( N_p \times N_p \) matrix and it has contribution from the volume integral term and the surface integral term on the right hand side of (19): \( \bar{G}_k = G^{vol}_k + G^{surf}_k, G^{vol}_k = [S^x_k \ S^y_k \ S^z_k]^T, G^{surf}_k = [L^x_k \ L^y_k \ L^z_k]^T \), where

\[
S^\nu_k(i, j) = -\int_{\Omega_k} \frac{d\ell_i(\mathbf{r})}{d\nu} \ell_j(\mathbf{r}) dV
\]

and

\[
L^\nu_k(i, j) = \frac{1 + \text{sign}(\hat{\beta} \cdot \hat{n})}{2} \theta_k(j) \int_{\partial \Omega_{kk'}} \hat{n}_\nu(\mathbf{r}) \ell_i(\mathbf{r}) \ell_j(\mathbf{r}) dS.
\]

Here, \( \partial \Omega_{kk'} \) denotes the interface connecting element \( k \) and \( k' \), \( \theta_k(j) \) is defined to select nodes on the interface

\[
\theta_k(j) = \begin{cases}
1, & \mathbf{r}_j \in \Omega_k, \mathbf{r}_j \in \partial \Omega_{kk'} \\
0, & \text{otherwise}
\end{cases}
\]

\( \bar{G}_{kk'} \) corresponds to the surface integral term [in (19)] involving unknowns from neighboring elements of the current element \( k \), \( \bar{G}_{kk'} = [\bar{L}_k^x \ \bar{L}_k^y \ \bar{L}_k^z]^T \), where

\[
L^\nu_{kk'}(i, j) = \frac{1 - \text{sign}(\hat{\beta} \cdot \hat{n})}{2} \theta_{kk'}(j) \int_{\partial \Omega_{kk'}} \hat{n}_\nu(\mathbf{r}) \ell_i(\mathbf{r}) \ell_j(\mathbf{r}) dS.
\]
Similarly, $\bar{C}_k$ is contributed by the fourth term (the volume integral) and the fifth term (the surface integral) on the right hand side of (18): 

$$\bar{C}_k = \bar{C}_k^{\text{vol}} + \bar{C}_k^{\text{surf}},$$

where

$$\bar{C}_k^{\text{vol}}(i, j) = \sum_\nu - \int_{\Omega_k} v_\nu(r) \frac{df_i(r)}{d\nu} \ell_j(r) dV$$

and

$$\bar{C}_k^{\text{surf}}(i, j) = \theta_k(j) \oint_{\partial \Omega_k} \left( \frac{1}{2} \sum_\nu \hat{n}_\nu(r) v_\nu(r) + \alpha(r) \right) \ell_i(r) \ell_j(r) dS.$$ 

$\bar{C}_{kk'}$ corresponds to the last surface integral term \(\text{in (18)}\) involving unknowns from neighboring elements,

$$\bar{C}_{kk'}(i, j) = \theta_{k'}(j) \oint_{\partial \Omega_{k'}} \left( \frac{1}{2} \sum_\nu \hat{n}_\nu(r) v_\nu(r) - \alpha(r) \right) \ell_i(r) \ell_j(r) dS.$$ 

$\bar{B}_n^k$ and $\bar{B}_q^k$ are contributed from the force term and boundary conditions (where element $k'$ does not exist) and are expressed as

$$\bar{B}_n^k(i) = \int_{\Omega_k} R(r, t) \ell_i(r) dV + \oint_{\partial \Omega_k \cap \partial \Omega_{k'}} f_R(r) \ell_i(r) dS$$

$$+ \oint_{\partial \Omega_k \cap \partial D} \hat{n}(r) \cdot v(r) f_D(r) \ell_i(r) dS$$

$$\bar{B}_q^k(i, \nu) = \oint_{\partial \Omega_k \cap \partial D} \hat{n}_\nu(r) f_D(r) \ell_i(r) dS.$$ 

For the time discretization of (22), an explicit third-order total-variation-diminishing (TVD) Runge-Kutta method [30] is used to incorporate with the high-order accuracy of the spatial discretization. With initial values $n(r, t = 0)$ being zero, $\bar{N}_k$ is iterated step by step in time. By using the explicit scheme, we implement an MPI-parallelized solver which does not involve solving any linear system in the time iteration. Meanwhile, from (22), we can see $\bar{Q}$ is a local variable which only needs to be defined as a temporary array of size $N_p$ and is flushed repeatedly when looping over elements. For this reason, this scheme is called local DG method.

The time-dependent Maxwell equations is solved with the nodal DG method [19]. Equations (10) and (11) are written in the conservation form

$$\bar{Q}(r) \partial_t \bar{q}(r, t) + \nabla \cdot \bar{F}(r, t) = \bar{s}(r, t)$$

where

$$\bar{Q}(r) = \begin{bmatrix} \varepsilon(r) & 0 \\ 0 & \mu(r) \end{bmatrix}, \bar{q}(r, t) = \begin{bmatrix} E(r, t) \\ H(r, t) \end{bmatrix},$$

$$\bar{s}(r, t) = \begin{bmatrix} -J(r, t) \\ 0 \end{bmatrix}, J(r, t) = J_e(r, t) + J_h(r, t)$$
and the flux vector is defined as

\[ \tilde{F}(r, t) = [\tilde{F}^x(r, t), \tilde{F}^y(r, t), \tilde{F}^z(r, t)]^T, \]

\[ \tilde{F}^\nu(r, t) = \begin{pmatrix} -\nu \times H(r, t) \\ \nu \times E(r, t) \end{pmatrix}, \nu \in \{x, y, z\}. \]

Discretizing the simulation domain into \( K \) elements, testing (23) with Lagrange polynomials on each element, and applying the divergence theorem twice yield the strong form

\[ \int_{\Omega_k} \tilde{Q}(r) \partial_t \tilde{q}_k(r, t) \ell_i(r) dV = -\int_{\Omega_k} \nabla \cdot \tilde{F}_k(r, t) \ell_i(r) dV + \int_{\partial\Omega_k} \tilde{F}_k(r, t) \ell_i(r) dS + \int_{\Omega_k} \tilde{s}_k(r, t) \ell_i(r) dV \]

(24)

where the subscript “k” denotes that the corresponding variable is defined locally on element \( k \). To recover a meaningful global solution, the local solutions are required to be identical on the interface between two neighboring elements, which is guaranteed by the uniquely defined numerical flux \( \tilde{F}^*(r, t) \) on the interface. For Maxwell equations, which belongs to hyperbolic problems (with real and distinct characteristic paths), solving the Riemann problem using the Rankine-Hugoniot condition yields the upwind flux, which leads to the expression

\[ \hat{n} \cdot (\tilde{F} - \tilde{F}^*) = \begin{pmatrix} F^E \\ F^H \end{pmatrix} = \begin{pmatrix} \hat{n} \times (\hat{n} \times [E] - Z^+ [H])/(2(Z)) \\ \hat{n} \times (Y^+ [E] + \hat{n} \times [H])/(2(Y)) \end{pmatrix} \]

where the average and jump operators are the same as those defined before, \( Z \) and \( Y \) are wave impedance and wave admittance, respectively. Here, the variables are defined on element surfaces and their explicit dependency on \( r \) and \( t \) is dropped for simplicity of notation. On boundaries where the neighboring unknowns are not defined, the numerical flux is assigned according to the boundary conditions. That is, on perfect electric conductor (PEC) boundaries, \( \hat{n} \times [E] = 2\hat{n} \times E^- \), \( \hat{n} \times [H] = 0 \), and, for absorbing boundary conditions (ABC), \( \hat{n} \times [E] = \hat{n} \times E^- \), \( \hat{n} \times [H] = \hat{n} \times H^- \). We note that, since the performance of ABC degrades rapidly with the angle of incidence, in addition to ABC, we also use the perfectly matched layers (PML) to truncate the simulation domain. Details of the PML implementation are referred to [31].

We expand \( E_k(r, t) \) and \( H_k(r, t) \) with Lagrange polynomials \( \ell_i(r) \)

\[ E_k^\nu(r, t) \simeq \sum_{i=1}^{N_p} E_\nu(r_i, t) \ell_i(r) = \sum_{i=1}^{N_p} E_k^{\nu,i}(t) \ell_i(r) \]

(25)

\[ H_k^\nu(r, t) \simeq \sum_{i=1}^{N_p} H_\nu(r_i, t) \ell_i(r) = \sum_{i=1}^{N_p} H_k^{\nu,i}(t) \ell_i(r) \]

(26)

where \( r_i \) denotes the location of interpolating nodes, \( \nu \in \{x, y, z\} \) denotes the components of vectors in the Cartesian coordinate system. \( E_k^{\nu,i}(t) \) and \( H_k^{\nu,i}(t) \) are the unknown coefficients to be solved for. Substituting (25)
and (26) into (24) yields

\[ \varepsilon_k \bar{M}_k \partial_t \bar{E}_k^x = \bar{S}_k^y \bar{H}_k^y - \bar{S}_k^z \bar{H}_k^z + \bar{L}_k F_{k}^{E,x} - \bar{M}_k \bar{J}_k^x \]  

(27)

\[ \varepsilon_k \bar{M}_k \partial_t \bar{E}_k^y = \bar{S}_k^z \bar{H}_k^z - \bar{S}_k^x \bar{H}_k^x + \bar{L}_k F_{k}^{E,y} - \bar{M}_k \bar{J}_k^y \]  

(28)

\[ \varepsilon_k \bar{M}_k \partial_t \bar{E}_k^z = \bar{S}_k^x \bar{H}_k^x - \bar{S}_k^y \bar{H}_k^y + \bar{L}_k F_{k}^{E,z} - \bar{M}_k \bar{J}_k^z \]  

(29)

\[ \mu_k \bar{M}_k \partial_t \bar{H}_k^x = -(\bar{S}_k^y \bar{E}_k^y - \bar{S}_k^z \bar{E}_k^z) + \bar{L}_k F_{k}^{H,x} \]  

(30)

\[ \mu_k \bar{M}_k \partial_t \bar{H}_k^y = -(\bar{S}_k^z \bar{E}_k^z - \bar{S}_k^x \bar{E}_k^x) + \bar{L}_k F_{k}^{H,y} \]  

(31)

\[ \mu_k \bar{M}_k \partial_t \bar{H}_k^z = -(\bar{S}_k^x \bar{E}_k^x - \bar{S}_k^y \bar{E}_k^y) + \bar{L}_k F_{k}^{H,z} \]  

(32)

where \( \bar{E}_k^\nu = [E_k^{\nu,1}(t),...,E_k^{\nu,N_p}(t)]^T \) and \( \bar{H}_k^\nu = [H_k^{\nu,1}(t),...,H_k^{\nu,N_p}(t)]^T \) are elemental unknown vectors, \( \bar{J}_k^\nu = [J_k^{\nu,1}(t),...,J_k^{\nu,N_p}(t)]^T \), \( J_k^{\nu,1}(t) = J_\nu(r,t) \) are the current density vectors, \( F_{k}^{E,\nu} \) and \( F_{k}^{H,\nu} \) are the \( \nu \) components of \( \mathbf{F}_k^{E} \) and \( \mathbf{F}_k^{H} \), respectively. The mass matrix \( \bar{M}_k \), stiff matrices \( \bar{S}_k^\nu \), and lift operator \( \bar{L}_k \) are defined as

\[ \bar{M}_k(i,j) = \int_{\Omega_k} \ell_i(r)\ell_j(r) dV \]

\[ \bar{S}_k^{\nu}(i,j) = \int_{\Omega_k} \ell_i(r)\frac{d\ell_j(r)}{d\nu} dV, \nu \in \{x,y,z\} \]

\[ \bar{L}_k(i,j) = \int_{\partial\Omega_k} \ell_i(r)\ell_j(r) dS \]

respectively. Here, \( \varepsilon(r) \) and \( \mu(r) \) are assumed constant in each element. The semi-discretized system (27)-(32) is solved with a low-storage five-stage fourth order Runge-Kutta method [19].

C. Discussion

It is worthwhile to remark the approximations used in the above models. First, since the static electric field is two orders of magnitude stronger than the transient field, the transient electric field is ignored in the field-dependent mobility model [7], [8]. Second, in Maxwell equations, the frequency-dependency of permittivity is ignored because of the relatively narrow bandwidth (less than 1%) of the optical pump used in practice. Third, the generation rate is simply considered as being proportional to the optical power density. Although this has been widely used in optoelectronic devices [8], [12], [15], [16], [25], a more strict treatment should consider the frequency-dependency of the optical absorption regarding to real material responses (including the photoelectric effect) and take into account the absorption of optical fields. Nevertheless, since the absorption is very weak, most optical wave energy is reflected or leaks out of the device. Thus, this simplified generation model performs very well in real devices [8], [12], [15], [16], [25]. Lastly, when eliminating the DC components from the Maxwell-DD system, the steady-state solution is assumed to be valid throughout the photocarrier generation process. Indeed, the optical pump only induces a small perturbation to the original biased state of the PCD device. The peak photocarrier densities are generally at least four orders of magnitude smaller than the doping concentration, which justifies the last assumption.
III. Numerical Examples

A. Conventional PCD Simulation

To validate the proposed solvers, we first model a conventional face-to-face dipole PCD. Because of the relative simple structure of this device, the scattering of the pumping wave is dominated by the reflection at the air-semiconductor interface. Such that the space-time varying optical field can be well approximated with an analytical expression. In [7], an analytical generation rate is used in an FDTD-based approach and the reported results match with experiments well. Similar results have been obtained in an FEM-based approach [15], [16] using approximated pulse shape function. In our multiphysics approach, we generate the pumping laser with an aperture source, such that we can directly model the propagation and scattering of the pumping light. This provides us the capability of modeling dynamic light-scattering/carrier-generation process in complex structures. Nevertheless, for this conventional device with relatively simple scattering, we expect to get similar results as those in [7], [15], [16].

As is done in [15], [16], here we focus on the photocurrent generation process and only consider the central gap region of the device. The device is depicted in Fig. 2. Since the gap region is invariant along the lateral z-direction, and the size in z-direction is much larger than that in x- and y- directions, the device can be modeled with a two-dimensional cross section in the x-y plane. Transverse magnetic (TM) polarization (with in-plane electric field components) laser is used to pump the device. The physical parameters are listed in Table. I.

1) Boundary conditions: Appropriate boundary conditions should be imposed with respect to the physical setup. The setup of the simulation domain is shown in Fig. 3. In both the steady-state and the transient stage modeling, the
DD equations are only considered in the photoconductive semiconductor layer. Consider the boundary conditions for DD equations, Poisson equation, and Maxwell equations separately:

(1) DD equations

On electrodes, the metal contacts are considered as ideal Ohmic contacts. Dirichlet boundary conditions can be derived using the local charge neutrality [26], [28], \( n_e = (C + \sqrt{C^2 + 4n_i^2})/2, \)
\( n_h = n_i^2/n_e. \)

On semiconductor-insulator interfaces, no carrier spills out of the interfaces. This corresponds to the homogeneous Robin boundary condition [28], \( \mathbf{n} \cdot \mathbf{J}_{e(h)} = 0. \)

(2) Poisson equation

On electrodes, considering ideal Ohmic contact, Dirichlet boundary conditions should be imposed [26], \( \varphi = V_{\text{external}} + V_{\text{built}} - V_{\text{in}}, V_{\text{built}} - V_{\text{in}} = V_T \ln (n_e^*/n_i). \)

On outer truncation boundary, the homogeneous Neumann boundary, \( \mathbf{n} \cdot \nabla \varphi = 0, \)

is used. This is justified by the converging test, i.e., requiring the truncation boundary is far enough from the device such that moving the boundary does not influence the solution near the device.

(3) Maxwell equations

The simulation domain is truncated with PML [31] combined with ABC. All internal material interfaces are treated naturally in the DGTD formulation. Drude model is used to model the metallic electrodes [32].

2) Scale analysis: For multiphysics modelling, because of the multiscale feature, it is crucial to understand all characteristic scales in the device and discretize the structure with respect to the limiting factors. The relevant length scales and time scales in PCDs are summarized below.

(1) Length scales

The length scales in PCDs are listed in Table. II. The structure feature sizes can be handled by the mesh generator. For conventional PCDs, this factor is not important because of the simplicity of the structure. To resolve the EM wave period, \( 0.2\lambda \) is used to estimate the corresponding mesh requirement, where \( \lambda \) is the wavelength of EM waves. The Debye length, \( \sqrt{2\varepsilon/(\mathbf{q}n_e)}, \) signifies the carrier density variations in space [26]. Because of the carrier
TABLE II

| Quantity                  | Required mesh size (nm) |
|---------------------------|-------------------------|
| Structure feature size    | $\sim 10^2$             |
| Pumping light wavelength  | $\sim 10^2$             |
| THz radiation wavelength  | $\sim 10^6$             |
| Debye length              | $\sim 10^2$             |
| Peclet number limit       | $\sim 10$              |

TABLE III

| Quantity                        | Required time step size (ps) |
|---------------------------------|------------------------------|
| CFL (Maxwell equations)         | $\sim 10^{-7}$              |
| CFL (DD drift term)             | $\sim 10^{-6}$              |
| CFL (DD diffusion term)         | $\sim 10^{-6}$              |
| Relaxation time                 | $\sim 10^{-2}$              |

generation, a maximal achievable carrier density should be used to estimate this length. Another limiting factor stemmed from the convection-diffusion problem is the Peclet number [33], which is required to be smaller than 1 to ensure stability. Consequently, the local mesh size is required to be smaller than $2D_c/|\mu_c E|$. Since the electric potential distribution is relatively smooth in this system, Poisson equation does not limit the mesh size.

(2) Time scales

Time scales give constraint on the time step size used in the transient solver. Table. III lists time step size limitations according to different terms. Basically, there are three CFL conditions, corresponding to Maxwell equations [19], and the convection and diffusion terms of DD equations [34], [35], respectively. The time step size required by CFL conditions are estimated using the mesh size resulted from the length scale analysis. Another important time scale is the relaxation time, which signifies the response speed of carriers to the applied electric fields. The EM wave periods are not listed because they are much larger than the CFL condition resulted from Maxwell equations. As we can see from Table. III, the CFL condition from Maxwell equations is the limiting factor. Since the carrier density changes slowly, the DD equations can be updated with a larger time step size than Maxwell equations. In our simulation the time step size for Maxwell equations and DD equations are $10^{-7}\text{ps}$ and $5 \times 10^{-7}\text{ps}$, respectively.

3) Steady-state solutions: In the Poisson-DD solver, the domain is discretized with respect to the Peclet number limit inside the LT-GaAs layer, with a minimal mesh size of 10nm. In other regions, the maximal mesh size is 200nm. Fig. 4(a) and Fig. 4(b) show the steady-state electric field and electron density solutions, respectively. Since no corresponding steady-state solution has been reported, the solutions are compared with the FEM solutions obtained from the COMSOL semiconductor module [36]. In COMSOL, we chose the fully-coupled nonlinear solver and second order FEM for discretization. GLS is used in FEM for stabilization. Fig. 4 (c) shows the comparison at
Fig. 3. Steady-state solutions. (a) Static electric field (b) Electron density (c) Comparison of the electron densities solved from the proposed DG solver and COMSOL (GLS-FEM) at lines $y = 0$ and $y = 0.5 \mu m$.

$y = 0.5 \mu m$ and $y = 0$. The differences are two orders smaller than the solutions. The relative difference, defined as $\frac{\|n_e^{DG} - n_e^{FEM}\|_2}{\|n_e^{FEM}\|_2}$, is smaller than 0.1%, where $\|\|_2$ denotes L2 norm. In Fig. 4 (b), one can see that the electron density shows sharp boundary layers, which is a typical phenomenon in convection dominated convection-diffusion problems. The larger the Peclet number, the thinner the boundary layer, and the finer meshes...
Fig. 4. Transient solutions. (a) $|H_z(r,t)|$ at different time instants. The yellow dotted line indicates the laser source aperture. The gray box indicates the LT-GaAs region. (b) $n_e(r,t)$ at different time instants. (c) The photocurrent signal (solid blue) and the laser pulse (dashed red). The inset shows corresponding frequency spectra. The signals are normalized for comparison with [7].

are needed near the boundaries.

4) Transient solutions: With the steady-state solution, one can run various transient simulations with different excitation. The source aperture is located at $y = 0.8\mu$m, generating laser propagating from top to bottom. The intensity on the aperture has Gaussian distribution with beam width $3\mu$m.

To understand the response process in the transient stage, Fig. 4 (a) and (b) show $|H_z^s(r,t)|$ and $n_e^s(r,t)$ at several time instants, respectively. In correspondence, Fig. 4 (c) shows the signals of the laser pulse and the
generated photocurrent. Fig. 4 (c) also serves as the reference of time in the following discussion.

At $t = 0.05\,\text{ps}$, the pumping light arrives the semiconductor layer. Because of the high permittivity of LT-GaAs, a large part of the pumping energy is reflected, see the reflected wave above the air-semiconductor interface and behind the aperture. In the mean time, in the LT-GaAs layer, the laser energy entering the device is (partially) absorbed and carriers are generated near the air-semiconductor interface. At $t = 0.25\,\text{ps}$, the laser reaches its pulse peak and the electron density immediately increases to $\sim 10^{11}\,\text{cm}^{-3}$. The short pumping pulse passes quickly and, after $t = 0.5$, only some scattering fields reside in the high permittivity region due to internal reflection. During that time, the electron density keeps increasing until the pumping pulse decays to 20% of its peak value (at $t \approx 0.4\,\text{ps}$, see Fig. 4 (c)). After $t \approx 0.4\,\text{ps}$, $n_e^t(\mathbf{r}, t)$ decays slowly due to the recombination.

In the mean time, comparing the electron density distributions at different time instants, it can be clearly observed that electrons move toward the anode on the left side. The picture of holes (not shown) is similar but with holes moving toward the cathode on the right side with a lower speed. As expected, the resulted photocurrent shown in Fig. 4 (c) agrees that in [7] very well. Because of the simplicity of the single interface scattering, the recorded EM field intensity in the semiconductor layer has almost the same pulse shape as the pumping signal. That explains why the analytical generation rate [7] works very well.

We note that, although the proposed method can model both the photocurrent generation and the THz radiation, model two processes in one simulation simultaneously is computationally very expensive because of the scale differences between THz and optical waves. This challenge will be further addressed in our future work.

B. Plasmonic PCDs Simulation

To show the capability of the proposed approach, we present a plasmonic PCD example. The device geometry is shown in Fig. 5. In this example, the nanostructures are added in-between the gap of the electrodes. The metallic nanograting is modeled as a group of floating potentials [27] in Poisson equation. For the case of nanostructured electrodes, one can set the nanograting as a Dirichlet boundary with the potential value the same as the bias voltage added on the corresponding electrode. In the EM solver, the metal material is modeled with Drude model [32]. Other parameters are the same as those in the previous section. Meanwhile, the nanograting requires finer meshes near the metal blocks to correctly resolve the geometry and the plasmonic fields. Here the minimal mesh size is 3nm and the time step size is $0.3 \times 10^{-7}\,\text{ps}$, which result in $\sim 10^8$ time steps.

1) Steady-state solutions: Fig. 6 shows solution of the steady-state electron density, which is again compared with the COMSOL semiconductor module solution, see Fig. 6 (c). Excellent agreements are observed between the two solvers. Here, noticeable enhancements of the static electric field and carrier densities are observed near the gratings. Because of velocity saturation [8], the enhanced static field leads to a significant drop of mobility, which will further influence the transient response.

2) Transient solutions: Fig. 7 shows the transient solutions at different time instants. For comparison, we have used the same color range in Fig. 7 and Fig. 4 for each subfigure. An overall comparison of $|H^t_z(\mathbf{r}, t)|$ shown in Fig. 7 and Fig. 4 shows that the EM fields are much stronger in the plasmonic case. Clear plasmonic mode patterns can be observed at $t = 0.05\,\text{ps}$ and $t = 0.25\,\text{ps}$. Accordingly, the electron density in Fig. 7 is much higher and
shows inhomogeneous patterns. As time iteration goes on, electrons drift toward the anode. Fig. 7 (c) compares the photocurrent obtained in the plasmonic PCD and that obtained in the previous conventional PCD. The photocurrent is enhanced around 7 times in this design.

It is worthwhile to note that, although the motivation of introducing plasmonic structure is to enhance the photocarrier generation through the plasmonic modes, the assessment of the overall device performance is still difficult and the root cause of the performance limitation (such as the high-power saturation effect) is yet inconclusive [4], [24]. From this example it is observed that, along with the enhancement of optical fields, the local static electric field is also enhanced, where the latter effect greatly influences the space-dependent mobility [see (??)]. While the plasmonic modes help increasing the number of carriers that could potentially contribute to the photocurrent, the drift velocity (determined by the local electric field and mobility) is important because it influences the number of carriers that can finally reach the electrodes within the carrier life time. In experiments, it is difficult to obtain such detailed information inside the device. With the proposed numerical approach, we expect to assess device performances through numerical experiments.

IV. Conclusion

In summary, we have proposed a multiphysics framework for the simulation of plasmonic PCDs. The device is modeled in two stages and the underlying nonlinear couplings are fully considered. The nonequilibrium steady-state is solved with a nonlinear Poisson-DD solver and the transient stage is modeled in time domain with a Maxwell-DD solver. All equations are solved under a unified framework using the DG methods. With the discretization flexibility provided by DG, the multiscale features of the plasmonic PCDs can be modeled efficiently. The solvers are verified with a conventional PCD example through comparison with references. A plasmonic PCD example is presented to show the capability of the proposed framework for analyzing the complex physics involved in the optical-to-THz process.

Plasmonic PCDs involve different mechanisms that are responsible for the overall device performance, such as the nanostructure tailored bias electric field, the plasmonic modes, the carrier-screening effect, and the antenna radiation
Fig. 6. Steady-state solutions. (a) Static electric field (b) Electron density (c) Comparison of the electron densities solved from the proposed DG solver and COMSOL (GLS-FEM) at lines $y = 0$ and $y = 0.5\mu m$.

efficiency, etc. Studying the impact factor of those mechanisms, and, more importantly, the competition between them is difficult and expensive in experiments. The proposed numerical approach provides an efficient way to optimize those devices and further makes it feasible to analyze different mechanisms separately by controlling/interfering the physical parameters through numerical experiments. Finally, we want to remark that the proposed solver is applicable to similar semiconductor optoelectronic devices, such as photovoltaic-effect based devices.
Fig. 7. Transient solutions. (a) $|H_z(r, t)|$ at different time instants. The yellow dotted line indicates the laser source aperture. The gray box indicates the LT-GaAs region. (b) $n_e(r, t)$ at different time instants. (c) The photocurrent generated in the plasmonic PCD (red) in comparison with that in the conventional PCD (blue). The inset shows corresponding frequency spectra.

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