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Multiphysics Modeling of Plasmonic Organic Solar Cells with a Unified Finite-Difference Method

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Abstract—A multiphysics study carries out on plasmonic organic solar cells (OSCs) by solving Maxwell’s equations and semiconductor (Poisson, drift-diffusion, and continuity) equations simultaneously with unified finite-difference framework. Regarding the Maxwell’s equations, the perfectly matched layer and periodic boundary conditions are imposed at the vertical and lateral directions of OSCs to simulate the infinite air region and metallic grating electrode, respectively. In view of the semiconductor equations, the Scharfetter-Gummel scheme and semi-implicit strategy are adopted respectively in the space and time domains. To model the bulk heterojunction OSCs, the Langevin bimolecular recombination and Onsager-Braun exciton dissociation models are fully taken into account. The short-circuit current, 

\[ J_{sc} = \text{incident photon power} \]

is the open-circuit voltage, FF is the fill factor, 

\[ \text{PCE} = \frac{J_{sc} \cdot V_{oc}}{P_{in}} \cdot \frac{1}{FF} \]

where \( J_{sc} \) is the short-circuit current, \( V_{oc} \) is the electrical properties of plasmonic OSCs, such as internal E-field concentration, plasmonics is one of enabling techniques for boosting the optical absorption of OSCs [3], [4], [5], [6]. The enhanced optical absorption substantially increases the generation rate of photocarriers and thus short-circuit current. The basic device physics of OSCs has been investigated in literatures [7], [8].

\[ \frac{1}{\epsilon_r} \frac{\partial}{\partial x} \left( \frac{1}{\mu_r} \frac{\partial E_z}{\partial x} \right) + \frac{1}{\epsilon_r} \frac{\partial}{\partial y} \left( \frac{1}{\mu_r} \frac{\partial E_z}{\partial y} \right) + k_0^2 E_z = 0 \]

(1)

Considering a two-dimensional OSC structure, the Maxwell’s equations can be decoupled into a TE and TM modes. The wave equations for TE and TM modes are respectively formulated as

\[ \frac{1}{\epsilon_r} \frac{\partial}{\partial x} \left( \frac{1}{\mu_r} \frac{\partial H_z}{\partial x} \right) + \frac{1}{\epsilon_r} \frac{\partial}{\partial y} \left( \frac{1}{\mu_r} \frac{\partial H_z}{\partial y} \right) + k_0^2 H_z = 0 \]

(2)

where \( k_0 \) is the wave number of incident light, and \( \epsilon_r \) and \( \mu_r \) are the relative permittivities and permeabilities, respectively.
Regarding non-magnetic optical materials, \( \mu_r = 1, \epsilon_r = n_r^2 \), and \( n_e \) is the complex refractive index of optical materials.

With the Yee lattice, the 2D finite-difference frequency-domain (FDFD) method [9] is utilized to characterize the optical properties of OSCs. As shown in Fig. 1, the five-point stencil is adopted for the FDFD method. The discretized forms for the TE \(( E_x)\) and TM \(( H_z)\) wave equations are respectively of the form

\[
2 \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) \frac{\Phi_0}{\epsilon} - k_0^2 \Phi_0 - \frac{\Phi_1 + \Phi_3}{\epsilon \Delta x^2} - \frac{\Phi_2 + \Phi_4}{\epsilon \Delta y^2} = 0 \tag{3}
\]

\[
2 \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) \frac{\Phi_0}{\epsilon} - k_0^2 \Phi_0 - \frac{\epsilon_1^{-1} + \epsilon_1^{-1} + \epsilon_3^{-1} + \epsilon_4^{-1}}{2 \Delta x^2} \Phi_1 - \frac{\epsilon_1^{-1} + \epsilon_2^{-1}}{2 \Delta y^2} \Phi_2 - \frac{\epsilon_3^{-1} + \epsilon_4^{-1}}{2 \Delta y^2} \Phi_3 - \frac{\epsilon_1^{-1} + \epsilon_2^{-1} + \epsilon_3^{-1} + \epsilon_4^{-1}}{4 \Delta y^2} \Phi_4 = 0 \tag{4}
\]

The incident Sunlight reflected by OSC devices converts to outgoing waves propagating into infinite air (or free-space) region. A perfectly matched layer (PML) absorbs the outgoing waves without spurious reflections and "perfectly" simulates unbounded wave propagations. The wave equation with the complex coordinate stretched PML is given by

\[
\frac{1}{s_r(x)} \frac{\partial}{\partial x} \left( \frac{1}{s_r(x)} \frac{\partial \Phi}{\partial x} \right) + \frac{1}{s_r(y)} \frac{\partial}{\partial y} \left( \frac{1}{s_r(y)} \frac{\partial \Phi}{\partial y} \right) + k_0^2 \Phi = 0 \tag{5}
\]

where \( s_r = 1 + i_0 \sigma / \omega \epsilon_0 \), \( i_0 \) is the imaginary unit, \( \epsilon_0 \) is the permittivity of free-space, and the conductivities \( \sigma(x) \) and \( \sigma(y) \) are non-zeros only within PML layers normal to the \( x \)- and \( y \)-axes, respectively. The optimized conductivities are chosen as

\[
\sigma_i = \frac{0.02}{\Delta} \left( \frac{2i - 1}{16} \right)^{3.7}, \quad i = 1, \ldots, 8
\]

\[
\sigma_{i+0.5} = \frac{0.02}{\Delta} \left( \frac{2i + 1}{16} \right)^{3.7}, \quad i = 0, \ldots, 8
\]

where \( \Delta = \Delta_x \) or \( \Delta = \Delta_y \) for the PML layers normal to the \( x \)- or \( y \)-axis, and \( i \) is the grid index of the eight-layer PML.

Regarding a periodic OSC device, the periodic boundary conditions need to be implemented. According to the Floquet or Bloch theorem, we have

\[
\Phi(x + P, y) = \Phi(x, y) \exp \left( i_0 k_0 \sin \theta \cdot P \right) \tag{6}
\]

\[
\Phi(x, y) = \Phi(x + P, y) \exp \left( -i_0 k_0 \sin \theta \cdot P \right) \tag{7}
\]

where \( P \) is the periodicity and \( \theta \) is the incident angle with respect to the \( y \)-axis.

B. Extraction of exciton generation rate

The exciton generation rate can be written as

\[
G(r) = \int_{0}^{800 \text{ nm}} \frac{2\pi}{h} n_c(\lambda) k_c(\lambda) c_0 |\mathbf{E}(r, \lambda)|^2 \Gamma(\lambda) d\lambda \tag{8}
\]

where \( h \) is the Planck constant, \( n_c = n_r + i_0 k_1 \) is the complex refractive index of the active polymer material, \( \mathbf{E} \) is the (optical) electric field that can be obtained by solving the Maxwell’s equations, and \( \Gamma \) is the solar irradiance spectrum of AM 1.5G. Moreover, the exciton generation rate is the average value of those for TE and TM polarizations.

C. Semiconductor equations

For studying electrical properties of OSCs, one should self-consistently solve the coupled nonlinear semiconductor equations (Poisson, continuity, and drift-diffusion equations) given by

\[
\nabla \cdot (\epsilon \nabla \phi) = -q(p - n) \tag{9}
\]

\[
\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot (-q \mu_n \nabla \phi + qD_n \nabla n) + QG - (1 - Q)R \tag{10}
\]

\[
\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot (-q \mu_p \nabla \phi - qD_p \nabla p) + QG - (1 - Q)R \tag{11}
\]

In the above, \( \epsilon \) is the dielectric constant of the polymer active material, \( q \) is the electron charge, \( \phi \) is the electrical potential, and \( n (p) \) is the electron (hole) concentration. Moreover, \( \mu_n (\mu_p) \) is the electron (hole) mobility, and \( D_n (D_p) \) is the electron (hole) diffusion coefficient accessible by Einstein relations and mobilities. Furthermore, \( J_n = -q \mu_n n \nabla \phi + qD_n \nabla n \) and \( J_p = -q \mu_p p \nabla \phi - qD_p \nabla p \) are respectively electron and hole current densities, and \( G \) is the excitation generation rate of Eq. (9) obtained with Maxwell’s equations. In addition, \( R \) is the bi-molecular recombination rate and \( Q \) is the field and temperature dependent exciton dissociation probability, which is a unique parameter for OSCs [10].

Using the Scharfetter-Gummel scheme in the spatial domain and using the semi-implicit strategy in the temporal domain [11], the 2D discretized forms of Eqs. (10) and (11) are respectively given by Eqs. (13) and (14), where \( B(x) = \frac{\sigma_1}{\sigma_{i+0.5}} \) is the Bernoulli function and \( U_i = \frac{k_0 T}{\sigma_1} \). It should be noted that the Gummel’s method has been incorporated in (13) to accelerate the convergence of the nonlinear semiconductor equations.

The boundary conditions play a key role in modeling electrical properties of plasmonic OSCs. The potential boundary condition for the Schottky contact is given by

\[
\phi = V_a - \frac{W_{in}}{q} \tag{12}
\]

where \( V_a \) is the applied voltage, and \( W_{in} \) is the metal work function. For the ohmic contact, the built-in potential is the potential difference between the highest occupied molecular orbital (HOMO) of donor and lowest unoccupied molecular orbital (LUMO) of acceptor. The Neumann (floating) boundary condition is used to truncate the left and right boundaries of OSCs, i.e.

\[
\frac{\partial \phi}{\partial N} = 0, \quad \frac{\partial n}{\partial N} = 0, \quad \frac{\partial p}{\partial N} = 0 \tag{13}
\]
of the plasmonic cell. From Fig. 2(d), the OSC to that of the standard OSC. The extremely dense exciton in the OSCs. The anode is assumed to be an ohmic contact while the infinite surface recombination velocity is assumed for the Schottky contact. It should be noted that the infinite surface recombination velocity is assumed for the Schottky contact.

III. RESULTS

The schematic standard and plasmonic OSC structures are shown in Figs. 2(a) and (b), respectively. The blend active layer of bulk heterojunction OSCs comprises a small bandgap donor of PBDTTT-C-T and an acceptor of PC$_{70}$BM. A silver rectangular-grating is introduced as the anode for the plasmonic OSC. Fig. 2(c) depicts the energy levels of active materials and electrodes. (d) The generation rate map of the plasmonic cell divided by that of the standard cell (in the active layer). The logarithmic scale is adopted.

Fig. 3 and Fig. 4 show the potential distribution, recombination rate, electron and hole current densities at the short-circuit condition for the standard and plasmonic OSCs, respectively. The geometric parameters are $d_1 = 30$ nm, $d_2 = 70$ nm, $d_3 = 30$ nm, $P = 300$ nm, $W = 150$ nm, and $H = 20$ nm. (c) The energy levels of active materials and electrodes. (d) The generation rate map of the plasmonic cell divided by that of the standard cell (in the active layer). The logarithmic scale is adopted.

The short-circuit current of the plasmonic cell is improved by 13% due to the plasmon enhanced photoabsorption as depicted in Fig. 5. The slightly increased open-circuit voltage

\[
\begin{align*}
\frac{1}{\Delta x} \epsilon_{d}^{i+1/2,j} \phi_{i+1,j}^{d+1} + & \frac{1}{\Delta y} \epsilon_{d}^{i-1/2,j} \phi_{i-1,j}^{d+1} + \frac{1}{\Delta x} \epsilon_{d}^{i,j+1/2} \phi_{i,j+1}^{d+1} + \frac{1}{\Delta y} \epsilon_{d}^{i,j-1/2} \phi_{i,j-1}^{d+1} \nonumber \\
- \left( \epsilon_{d}^{i+1/2,j} + \epsilon_{d}^{i-1/2,j} + \epsilon_{d}^{i,j+1/2} + \epsilon_{d}^{i,j-1/2} \right) \left( \frac{1}{2 \Delta x^2} + \frac{1}{2 \Delta y^2} \right) \phi_{i,j}^{d+1} - \frac{n_{i,j} + p_{i,j}^t}{U_t} \phi_{i,j}^{d+1} \nonumber \\
= q(\beta_{i,j}^t - \beta_{i,j}^f) - & \frac{n_{i,j}^t + p_{i,j}^t}{U_t} \phi_{i,j}^t
\end{align*}
\]
Fig. 3. The electrical results of the standard OSC at the short-circuit condition. (a) equipotential lines (V); (b) recombination rate with the logarithmic scale (m$^{-3}$s$^{-1}$); (c,d) electron and hole current densities (A/m$^2$). The color and arrow denote the amplitude and direction of the currents.

Fig. 4. The electrical results of the plasmonic OSC at the short-circuit condition. (a) equipotential lines (V); (b) recombination rate with the logarithmic scale (m$^{-3}$s$^{-1}$); (c,d) electron and hole current densities (A/m$^2$). The color and arrow denote the amplitude and direction of the currents.

in the plasmonic OSC may be attributed to the favorable hole transport. A lot of holes are generated around the grating anode and can be collected efficiently. The FF is defined by the maximum power output over the product of short-circuit current and open-circuit voltage. A significant 7% drop of the FF in the plasmonic cell is strongly confirmed by our multiphysics model. On one hand, the periodically-modulated metallic grating excites the concentrated plasmonic waves near the anode resulting in nonuniform photocarrier generation (Fig. 2(d)). On the other hand, the modulated anode boundary is responsible for inhomogeneous built-in potential and internal E-field distributions below ridge and troughs of the grating anode, which has strong effects on the photocarrier transport and collections.

IV. CONCLUSION

We have investigated the plasmonic OSC with the metallic rectangular-grating anode through the multiphysics solutions to Maxwell’s equations and semiconductor equations with unified finite-difference method. The grating anode induces nonuniform optical absorption and inhomogeneous internal E-field distribution. Thus uneven photocarrier generation and transport are formed in the plasmonic OSC leading to the dropped FF. The multiphysics modeling and understanding are fundamentally important for improving the performance of organic photovoltaics.

REFERENCES