Dipole emission modelling using TMM for solar cell and LED applications

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***Abstract*—An optical modeling approach employing the transfer matrix method (TMM) including internal sources has been described and implemented in the TiberCAD software. This method allows for the simulation of various optoelectronic devices. In particular, it has been employed to simulate a perovskite solar cell and investigate the effects of re-emission of absorbed photons. Additionally, the TMM is used to model a GaN light emitting diode (LED) with an internal light source.**

***Index Terms*—TMM, dipole, solar cell, LED**

I. INTRODUCTION

Optical modeling plays a crucial role in accurately studying LEDs and solar cells, enabling advancements in scientific research and facilitating effective design enhancements for practical applications. The transfer matrix method (TMM) has been extensively used to calculate the propagation of light from external sources in multi-layer structures, as demonstrated by [1]. However, TMM can also be applied to model dipoles within layers, known as internal sources. These internal sources can result from spontaneous emission in LEDs or the re-emission of absorbed photons in solar cells, often referred as photon recycling. Incorporating internal emission caused by photon recycling in solar cell simulations enables more precise modeling and optimization, ultimately pushing the efficiency of solar cells closer to their theoretical limits.

According to the theory of the transfer matrix method (TMM), the electric field of two consecutive layers within a multi-layer structure can be mathematically linked to each other using equation(1):

$$\begin{bmatrix} E_{i+} \\ E_{i-} \end{bmatrix} = L_i I_{i,i+1} \begin{bmatrix} E_{(i+1)+} \\ E_{(i+1)-} \end{bmatrix} \tag{1}$$

where $E_{i\pm}$ is the electric field in i layer and $-, +$ sign represent direction in which the respective wave is travelling. The matrix of the layer i L_i is named phased matrix:

$$L_i = \begin{bmatrix} e^{-jk_{zi}d_i} & 0 \\ 0 & e^{+jk_{zi}d_i} \end{bmatrix}, \tag{2}$$

where d_i is the thickness of the layer and the k_{zi} is complex wave vector along propagation direction, consistent with $k_{zi}^2 + k_r^2 = k_i^2$. Here, k_r is the radial wave-vector and k_i is the total wave-vector. Accordingly, the propagation angle can be defined as

$$\cos\phi_i = \frac{k_{zi}}{k_i} = \sqrt{1 - \frac{k_r^2}{(2\pi n_i)^2}}, \tag{3}$$

where n_i is the complex refractive index of the i-th layer. Note that ϕ_i can be complex.

The transmission matrix $I_{i,i+1}$ is defined as follows:

$$I_{i,i+1} = \begin{bmatrix} \frac{1}{t_i} & \frac{r_i}{t_i} \\ \frac{r_i}{t_i} & \frac{1}{t_i} \end{bmatrix} \tag{4}$$

The transmission and reflection coefficients t_i and r_i are calculated using Fresnel equations. To incorporate the internal emission of a dipole into the calculation, it is necessary to include a source term and apply it to the layer that contains the dipole. This can be achieved by utilizing the following equation:

$$\begin{bmatrix} A_+ \\ A_- \end{bmatrix} = \begin{bmatrix} E'_{s+} \\ E'_{s-} \end{bmatrix} - \begin{bmatrix} E_{s+} \\ E_{s-} \end{bmatrix} \tag{5}$$

The parameters $A_{-,+}$ are normalized source terms depending on dipole polarization and orientation[2]. E_s and E'_s are the extra electric-field components immediately before and after the dipole location, respectively. The electric field in each layer can be calculated using the equation mentioned above, while applying the appropriate boundary conditions, as described in more detail in [1]. Once the electric field distribution within the layer is obtained, it becomes possible to calculate the Poynting vector using

$$S_{zi}^{TE} = \Re\{n_i \cos\phi_i (E_{i+} + E_{i-})^* (E_{i+} - E_{i-})\} \tag{6}$$

$$S_{zi}^{TM} = \Re\{n_i \cos\phi_i^* (E_{i+} + E_{i-})^* (E_{i+} - E_{i-})\}. \tag{7}$$

II. PHOTON RECYCLING IN SOLAR CELLS

Photon recycling primarily affects the open-circuit voltage (Voc) of a solar cell, which can be quantified by

$$\Delta V_{oc} = -\frac{k_B T}{q} \ln(\eta_{ext}), \tag{8}$$

where k_B is the Boltzmann constant, q the elementary charge, T the temperature and η the external photoluminescence quantum efficiency (PLQE) [3]. That is, if the internally emitted photons cannot easily escape the cell ($\eta_{ext} < 1$), V_{oc} increases.

Internally emitted photons can escape the active layer through the escape cone. This escape probability is constrained by the factor $(1/4n^2)$, where n represents the refractive index. Assuming the presence of a perfect back reflector and a textured interface with air, the photon recycling effect in a common perovskite solar cell ($n = 2.34$) can increase V_{oc} by approximately $79.8mV$.

By applying the approach discussed earlier, a more precise escape probability can be calculated. Multiple dipoles, uniformly distributed along the active layer, are used to represent internal emission. By calculating the mean value of the escape probability for each dipole, the total escape probability is determined. On average, only approximately 5.76% of the emissions escape the active layer, resulting in a boost of $74mV$ in Open circuit voltage. The optical intensity of light resulting from both an external source and an internal source is depicted in Figure 1.

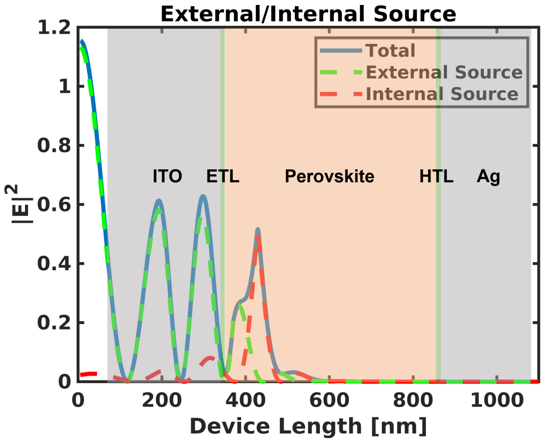

Fig. 1. Normalized poynting vector from 3 of the dipoled inside active layer of a common perovskite solar cell.

III. LED EMISSION

The TMM with an internal source proves to be a valuable tool for studying light propagation within LEDs, offering insights for optimizing out-coupling efficiency and emission patterns. To investigate these aspects, a simplified structure representing a GaN LED, shown in Fig. 2, was modeled using the TMM with an internal source. Figure 2 displays the Poynting vector distribution within the LED device, revealing the escape of light predominantly from the sapphire side, while also indicating a smaller fraction of light being absorbed in the silver layer.

The directivity of an LED is a significant parameter. It can be easily calculated by varying the emission angle of the dipole. The radiation pattern of the LED is depicted in Figure 3, providing a visual representation of the angular distribution of emitted light.

IV. CONCLUSIONS

The transfer matrix method with internal sources has been implemented and its applicability for the simulation of solar cells and LEDs has been demonstrated, studying the photon recycling effect and emission patterns. The model provides valuable insights for optimizing performance and design enhancements of such devices with low computational cost. Future work includes the selfconsistent coupling with the electrical device models.

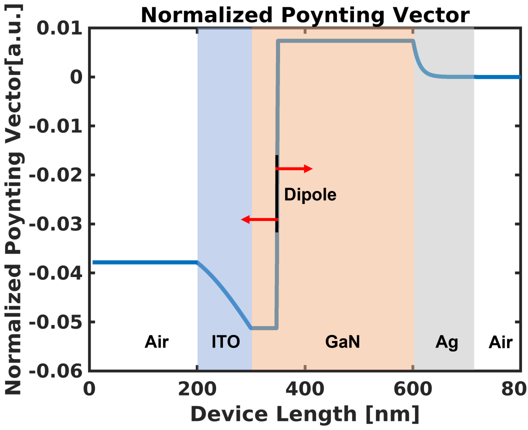

Fig. 2. Normalized Poynting vector distribution in a GaN LED using TMM with internal source.

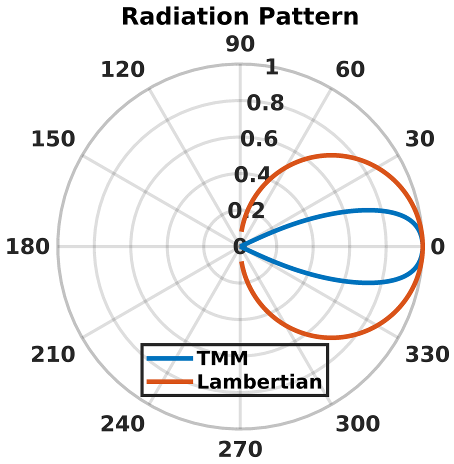

Fig. 3. Radiation pattern of a GaN LED compared to the Lambertian pattern.

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