Modeling the Impact of Light Scattering on Photon Recycling in Solar Cells and LEDs

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***Abstract*—A comprehensive 1D optical multiscale model combining coherent as well as incoherent light transport with support for incoherent light scattering is presented. The model is based on a detailed-balance conforming formulation of dipole emission and an incoherent net-radiation model, extended to scattering interfaces in the optical layer stack where various models can be used to compute the scattering matrices. Given its unified framework treating emission and absorption, this model excellently lends itself to the analysis of photon recycling and luminescent coupling effects in solar cells and LEDs and can be easily coupled to a drift-diffusion model to further analyze the full opto-electronic behavior of the device.**

***Index Terms*—photon recycling, scattering, opto-electronic modeling, solar cell, led**

I. Introduction

Photon management and efficient utilization of light play crucial roles in advancing the performance of modern solar cells and light-emitting diodes (LEDs). Indeed, light scattering has been implemented in LEDs to remove lossy waveguide modes and enhance the external quantum efficiency (EQE) [1], and practically all recent record-performing solar cells employ light scattering to enhance light absorption [2]. These designs therefore also largely impact photon recycling (PR). Recently, PR has seen again rising interest due to the excellent opto-electronic properties of lead-halide perovskite materials used in solar cells (single junction or perovskite-Si tandems) as well as perovskite LEDs (PeLEDs), where the strong optical absorption and small Stoke's shift give rise to PR and luminescent coupling (LC) resulting in increased open-circuit voltages (V_{oc}) for solar cells [3] and increased EQE for PeLEDs [4].

In order to accurately predict and analyze the opto-electronic behavior of modern solar cells and LEDs under consideration of PR effects, we extend our previously published theory [5], [6] of PR in purely coherent optical environments to the realm of optically thick layers and rough interface geometries where conservation of optical in-plane momentum $q_\parallel$ is broken. Still, this model is easily coupled to a Poisson-drift-diffusion solver to take the intricate interplay between electronic and photonic processes into account.

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II. Modeling Approach

A. Coherent Light Transport

The theory describing the fundamental coherent emission and light transport processes used as a basis for the present model has been discussed in [5]. For completeness the most important expressions are repeated here. The coherent optical environment is described completely by the dyadic Green's tensor for the transverse electric fields $\overleftrightarrow{G}$, from which a *generalized van Roosbroeck – Shockley* relation for internal emission to an arbitrary local photonic density of states (LDOS) can be derived, viz.

$$\mathcal{R}_{\mathrm{rad}}(z) = \int \mathrm{d}E_\gamma \, \frac{4E_\gamma^2}{\pi\hbar^3 c_0^2} n_r(z,E_\gamma)\kappa(z,E_\gamma) f_{\mathrm{BE}}(E_\gamma - \Delta\mu_{cv}(z)) \times \sum_\mu \int \frac{\mathrm{d}^2\vec{q}_\parallel}{(2\pi)^2} \Im\left[G_{\mu\mu}(\vec{q}_\parallel, z, z, E_\gamma)\right]. \quad (1)$$

Furthermore, the resulting coherent *reabsorption* rate can be calculated, as well as the *Poynting vector* for outcoupled modes (showing just TE component)

$$S_{\mathrm{z}}^{y}(z,E_\gamma) = \frac{4E_\gamma^2}{\hbar^3 c_0^2 \pi} \int \mathrm{d}z' \, n_r(z',E_\gamma)\kappa(z',E_\gamma) \times f_{\mathrm{BE}}(E_\gamma - \Delta\mu_{cv}(z'))\Im \int \frac{\mathrm{d}^2\vec{q}_\parallel}{(2\pi)^2} G_{yy}(\vec{q}_\parallel, z, z', E_\gamma) \times \left[\partial_z G_{yy}(\vec{q}_\parallel, z, z', E_\gamma)\right]^*. \quad (2)$$

In the above equations E_γ, n_r and κ are the photon energy, refractive index and extinction coefficients, respectively, and f_{BE} denotes the Bose-Einstein distribution function with quasi-Fermi level splitting $\Delta\mu_{cv}$.

B. Incoherent Light Transport and Scattering

Incoherent light transport is appropriately modeled using light intensities (energy fluxes) only, i.e. a ray-optical approach is taken. At each interface i, the upwards $I^\sigma_{\mathrm{i,b/c}}$ and downwards $I^\sigma_{\mathrm{i,a/d}}$ propagating fluxes are related by the reflectances R^σ_{i} and transmittances T^σ_{i}. The source terms $\hat{I}^\sigma_i$ result either directly from the coherent Pointing vector given in (2), possibly altered by the roughness of the emitting interface itself, or from the incoherent Poynting vector expression for incoherent emitters

$$\hat{S}_z^y(z, E_\gamma) = \frac{4E_\gamma^2}{\hbar^3 c_0^2 \pi} n_r(z, E_\gamma)\kappa(z, E_\gamma) f_{\mathrm{BE}}(E_\gamma - \Delta\mu_{cv}(z)) \times \Re \int \frac{\mathrm{d}^2\vec{q}_\parallel}{(2\pi)^2} \left[\frac{1}{4q_\perp(\vec{q}_\parallel, z, E_\gamma)}\right]. \quad (3)$$

The resulting linear system of equations for the fluxes at given $q_\parallel$,

$$I_{i,a}^\sigma = P_{i-1}^2 R_{i-2,i-1}^\sigma I_{i,b}^\sigma + P_{i-1} T_{i-2,i-1}^\sigma I_{i-1,a}^\sigma \quad (4a)$$

$$I_{i,b}^\sigma = \hat{I}_{i,b}^\sigma + T_{i-1,i}^\sigma I_{i,c}^\sigma + R_{i,i-1}^\sigma I_{i,a}^\sigma \quad (4b)$$

$$I_{i,c}^\sigma = P_i^2 R_{i+1,i}^\sigma I_{i,d}^\sigma + P_i T_{i,i+1}^\sigma I_{i+1,b}^\sigma \quad (4c)$$

$$I_{i,d}^\sigma = \hat{I}_{i,d}^\sigma + T_{i,i-1}^\sigma I_{i,a}^\sigma + R_{i-1,i}^\sigma I_{i,c}^\sigma \quad (4d)$$

with $P_i = \left|\mathrm{e}^{iq_{\perp,i}d_i}\right|^2$, can then be solved for all interfaces at once. Parameters $q_{\perp,i}$ and d_i are the complex out-of-plane momentum and propagation distance, respectively.

For flat interfaces, in-plane momenta are decoupled and the fluxes can be found for each $q_\parallel$ individually. If there are scattering interfaces present, they become coupled and I_i^σ become *vectorial* quantities with R_i^σ and T_i^σ becoming reflection and transmission *matrices* (BSDF), where all $q_\parallel$ have to be solved simultaneously. These matrices can be generated from simple analytic models up to full 3D ray-tracing simulations of the interface geometry.

III. Results

The model is compared in Fig. 1a) for an idealized situation where analytical solutions can be obtained. The reabsorption probability in the ray-optical regime for emission within a homogeneous MAPI slab in air with lambertian surfaces was computed for varying slab thickness and compared to the analytical model obtained in [7], using the refractive index of MAPI at $E_\gamma = 1.61\,\mathrm{eV}$. For a fixed outcoupling probability $p_e = 1/n_r^2$, strong agreement between model and simulation was obtained, while using angle-dependent Fresnel coefficients introduces a deviation toward larger thicknesses.

Fig. 1b) shows the reabsorption rate and energy flux profiles for a thin-film PeLED structure on a glass substrate with a polished or rough surface. The rough scattering surface of the glass substrate indeed leads to a higher outcoupling efficiency of the PeLED as can be observed from the increased energy flux propagating to the left. This in turn leads to a smaller reabsorption rate in the active layer itself, where the difference is however small ($\approx -18\%$) since a large portion of the reabsorbed light stems from coherent guided modes which are unaffected by the rough glass.

IV. Conclusions

An extended optical model for analysis of photon recycling in opto-electronic devices with support for incoherent light scattering is presented. The combination of coherent and incoherent light transport with light scattering allows for application of the model for perovskite-Si tandem solar cells, where usually the Si wafer is fully textured, or PeLEDs with scattering light-outcoupling structures. The direct usability of the calculated optical rates in a Poisson-drift-diffusion model further extends the analysis capabilities to the electronic transport regime to investigate the behavior of the main device key figures.

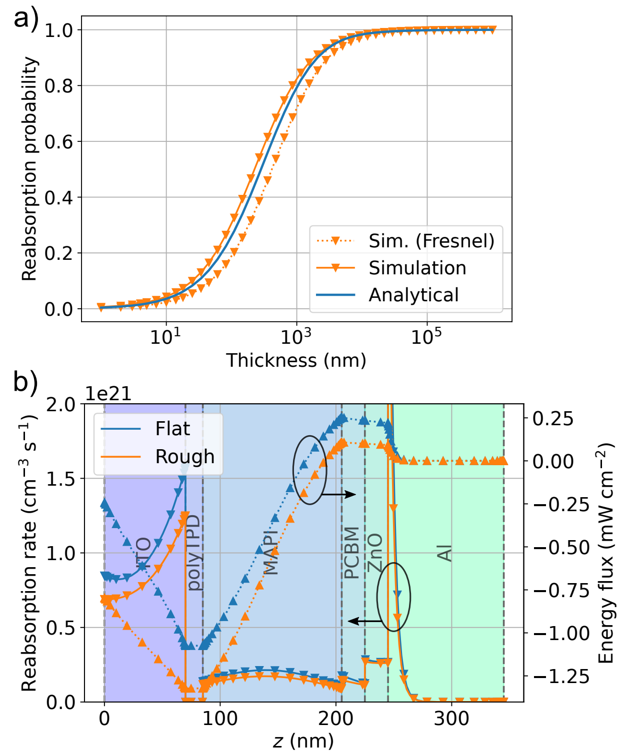

Fig. 1. a) Reabsorption probability of a homogeneous MAPI slab with lambertian surfaces in air with varying thickness, compared to the analytical model of [7]. b) Reabsorption rate and energy flux profiles for a PeLED on a glass substrate with flat or rough surface (glass not visible in plot).

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