Mixed-Level Simulation of Opto-Electronic Devices

(Invited Paper)

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Abstract- Presented here are two important devices that cannot be modeled accurately and/or tractably by a single simulation technique. Simulation flows to address each device are presented. The first is a patterned Light Emitting Diode (LED), the optical modeling of which requires a mixed-level simulation approach combining FDTD (or RCWA) and Ray Tracing. The second is a CMOS Image Sensors (CIS), which requires process, optical and electrical simulation techniques.

I. INTRODUCTION

Modern OLED/LEDs contain a variety of geometric structures that exist on very disparate size-scales. Ray optics based techniques, such as Monte Carlo ray-tracing (RT), are appropriate to analyze thick planar layers and packaging structures. However, these techniques fail to address the subwavelength geometric features including coherent effects like diffraction and interference. These may instead be addressed with rigorous electromagnetic (EM) wave optics based techniques, such as finite-difference time-domain (FDTD) and rigorous coupled wave analysis (RCWA). However, these rigorous techniques have difficulty in analyzing the larger structures due to computational limitations. A mixed-level simulation approach, presented in Section II., is required to circumvent the limitations of the individual numerical techniques. CMOS image sensors [1] are another important device category that cannot be properly analyzed without considering multiple techniques. These require optical and electrical simulations, as well as process simulation for accurate determination of structure and doping profile based on growth conditions. Section III presents such an example and an appropriate simulation flow.

II. MIXED-LEVEL OPTICAL SIMULATION OF LEDs

A. Simulation Flow

The mixed-level simulation flow [2] uses rigorous techniques to model the regions of a structure where coherence is important, such as interface gratings or thin film stacks. Each set of resultant scattering information is used to create a Bi-Directional Scattering Distribution Function (BSDF) which can be used as a surface property within RT simulations to model the overall device performance. Furthermore, if needed an incoherent source for the RT simulation maybe constructed from multiple FDTD simulations. An example of this flow for an OLED is shown in Fig 1 (a) where the thin film stack (TFS) is reduced to an incoherent source emitting in glass substrate and a BSDF. A second BSDF, representing a Moth's eye pattern at the glassair interface, is calculated via RCWA. These two BSDF's and the source are then incorporated into the simplified structure, Fig 1(b), which is now appropriate for modeling via RT (see [1] for example simulation results).



Fig. 1. (a) OLED structure showing where the EM (FDTD, RCWA) methods were applied to generate data for ray-tracing model. (b) Simplified OLED structure used for ray-tracing simulation where the EM results were used.

B. Example structure and Result

To demonstrate the significance of the mixed-level approach we studied the extraction ratio from a collimated source between a 1D large period rectangular surface grating and a back reflector (Fig. 2(a)) using commercial tools [3]. For small period gratings (Period/ λ <10-50) an RT approach would be expected to have limited accuracy, while for large period gratings (Period/ λ >50), it would be expected to agree with more rigorous techniques. However, coherent effects, in structures such as those in Fig 1(a) and 2(a), play an important role even for large period gratings. Fig 2(b) compares the simulated extraction ratios from RT alone and the Mixed-Level approach, and significant differences can be seen [4].



Fig. 2. (a) 1D rectangular surface grating with back reflector. The duty cycle for the rectangular grating was 0.5, φ is the collimated launch angle. (b) Light extraction ratio into air, with Period/ $\lambda \sim 71$, calculated via the two simulation methods mixed-level (solid with circles) and ray-tracing (dashed with squares)

III. OPTO-ELECTRONIC SIMULATION OF CIS

A. Simulation Flow

The complete simulation flow for modeling a CMOS Image Sensor should include process, optical, and electrical simulations. An example of such a flow is shown in Fig 3 for a simple Back Side Illuminated (BSI) CIS device (Fig 3(a)). Process simulation is necessary to create a realistic device structure including diffusion, implantation, oxidation, etching, deposition, and silicidation [5]. The output of the process simulator includes a geometry and doping profile (Figs 3 (a, b)) for the electrical simulator [5]. The complex refractive index (CRI) (Fig 3 (c)) can be obtained either directly from the geometry or through an unilluminated electrical simulation which can include the effect of carriers. Using the CRI obtained from the previous step, optical simulations are then performed using FDTD resulting in a spatially dependent electric field (Fig 3(d)) and absorbed photon density (APD) (Fig 3(e)). Finally, the structure obtained from the process simulation and the APD obtained through the optical calculations are used by the transport simulator [5] to determine the steady-state (e.g. electrostatic potential Fig 3(f)) and transient electrical responses of the device (Fig 4).



Fig. 3. Complete simulation flow for CIS modeling: (a) BSI CIS structure (b) Net doping concentration from Process simulation (c) Refractive Index profile (d) electric field, |E| (e) Absorbed photon density from FDTD (f) Electrostatic potential from electrical simulation. Note that cross-sections shown in b through f are taken at $x=1.2\mu m$ (middle of lens).

B. Example structure and Result

As an example we simulate the performance of a single pixel BSI CIS device under dark conditions as well as under illumination at a wavelength of 550nm. The size of the pixel used was $2x2x5 \ \mu\text{m}^3$ and several of the features are sub-wavelength, see Fig 3(a). Therefore, the predictive optical simulation of a CIS requires the description of diffraction and interference effects through rigorous EM simulations (e.g. FDTD). The process, optical and electrical simulations were performed as described in the previous section. In the electronic simulation the pixel is illuminated between 10-110 µs. During this period, the doping well is re-populated by

photo-generated carriers. The transfer gate is biased with a transient trapezoidal pulse (dash line in Fig 4). The high voltage part opens the gate, depleting the active silicon photodiode region. Note that even without illumination there is initial charge in the doping well which is transferred out on the first rising edge of the transfer gate pulse (dash -dot line in Fig 4). During each transfer gate cycle, a linear drop in the number of carriers for $V_{TX} = 2.5$ V indicates a constant flow of electron current out of the doping well (solid line in Fig 4). During the low voltage period, 40-80µs, the doping well is repopulated by the incident light and reaches saturation.



Fig. 4. Transient characteristics showing the applied transfer gate voltage (dash line), electrons generated under illuminated (solid line) and unilluminated (dash-dot line) conditions.

The above example demonstrates the simulation flow applied to a CIS but the methodology can also be used for modeling other opto-electronic devices such as modulators and photodetectors.

IV. CONCLUSION

We have presented a mixed-level simulation approach and a hybrid approach and associated examples demonstrating the importance of each. It was shown that certain problems would be intractable or subtle effects missed if less thorough approaches were used.

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