Advanced Optoelectronic Technologies : Device Optimization and Securing Production with Predictive Simulation Tool-chains

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***Abstract*—The continuous evolution of semiconductor consumer electronic global market, including autonomous systems, augmented and virtual reality (AR/VR), and energy-efficient technologies, necessitates the development of advanced optical sensing solutions. These applications demand innovative optoelectronic devices, such as RGB and near-infrared (NIR) image sensors, but also time-of-flight optical sensors and multi-spectral ambient light sensing. Sequential 3D stacking, hybrid bonding and pixel size shrinkage has revolutionized CIS design, enabling differentiated pixel architectures that meet the demands of emerging applications and hold significant promise for the next generation of optical sensors. Metasurfaces, advanced optical filters and surface structuration technologies also further expands the capabilities of optical sensors, paving the way for high-resolution, energy-efficient imaging and all-in-one sensing solutions from visible to NIR wavelengths.**

This paper presents a comprehensive overview of the recent state-of-the-art advancements in CMOS image sensors (CIS), emphasizing their technological breakthroughs, challenges, and future directions. We highlight the importance of predictive simulation tools to address these challenges and support the integration of advanced CIS into these complex systems. Advanced multi-physics simulation capabilities are required to model light propagation, carrier transport and material properties, but also for the integration of optical devices into larger system modules. Additionally, neural-network-based approaches are gradualy emerging to emulate and optimize large meta-surface optical systems, but also to make possible the optimization of new optical enablers such as in-pixel embeded meta-surface color routers.

I. Introduction

Emerging applications in automotive, industrial, and consumer electronics sectors demand differentiated pixel architectures to achieve high-resolution imaging, depth sensing, and low consumption [1], [2]. Traditional image sensors are being enhanced with 3D integration, advanced structured interfaces, interference filters, and time-of-flight (ToF) technologies. These advancements enable e.g. precise 3D depth mapping and obstacle detection, which are critical for autonomous systems and AR/VR applications. The development of innovative optoelectronic devices relies on a synergistic combination of advanced technologies and predictive simulation tools. Main innovative technological bricks are summarized in Section II, highlighting the challenges and optimization strategies. Simulation tools and modelling methodologies are presented in Section III, with key results.

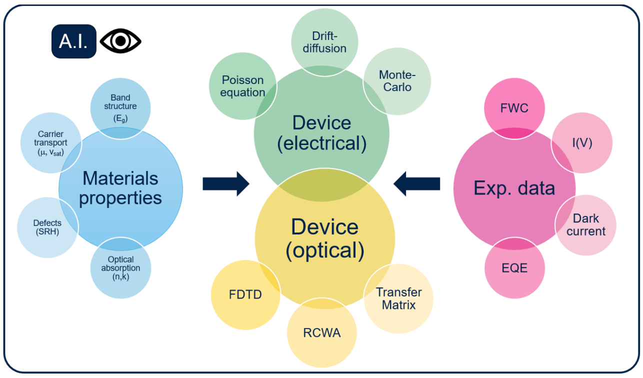

Fig. 1. Overview of the simulation framework, encompassing process, materials, and device simulation. Artificial intelligence (AI) supervision and optimization enhance efficiency in individual components and enable a unified multi-scale approach.

II. Advanced Technology

A. Sequential 3D Stacking: A Technological Breakthrough

3D stacking and backside illumination (BSI) technologies have emerged as a transformative technology in CIS development, enabling the integration of high-performance photodiodes with advanced CMOS processing layers [3]. This approach combines the advantages of dedicated pixel technology optimized for high quantum efficiency (QE) and low noise with high-density, low-power CMOS layers for digital and analogue processing. Key benefits of 3D stacking include; i) reduced die size through efficient use of silicon technology, ii) enhanced performance via improved QE, modulation transfer function (MTF), and reduced crosstalk, iii) scalability enabled by hybrid bonding techniques with fine pitch interconnects down to 1 µm.

Despite its advantages, 3D stacking presents several challenges:

- Achieving reliable hybrid bonding at pitches below 1 µm requires advanced process control and materials engineering.
- Thermal budget management must accommodate the constraints of top-layer processing.
- Innovations in BSI stack design and small pitch pixels doping are critical for minimizing dark current and hot pixels.

Additionally, sequential 3D stacking offers a promising pathway for further miniaturization and performance enhancement while maintaining cost efficiency. This approach involves the integration of multiple tiers, each optimized for specific functions (see Fig. 2): Tier 1: Light-sensitive pixel areas with high QE and low noise, Tier 2: Analogue processing and memory for feature extraction or GS pixel transistors, Tier 3: Advanced CMOS logic for data processing and storage.

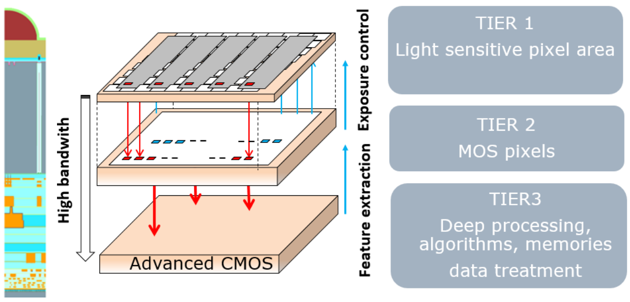

Fig. 2. (Left) Process Emulation of a 3D stacked pixel. (Right) schematic of sequential 3D stacking technology.

B. Quantum Efficiency Enhancement

Under-display and low-light applications are driving the development of high-sensitivity solutions for image sensors. On one hand, for performance in the NIR wavelength, the technological innovations include: i) diffractive structure to increase light travel and enhance QE [6], ii) deep trench optimization to reduce crosstalk and improve MTF [7]. On the other hand, in the visible wavelengths, the technology breakthroughs involve: i) low-index materials engineering for isolation walls, ii) improved organic resists for small pitch filters, iii) optimized broadband anti-reflective coatings, iv) novel architectures (e.g. QuadBayer and Nonacells patterns) [9]. In-pixel meta-surfaces for colour routing have also emerged in the literature thanks to advanced optimization [5].

C. SPADs for Direct Time-of-Flight Applications

SPADs are critical components for direct time-of-flight (dToF) sensors, offering high sensitivity and precise timing resolution for distance measurements. Key advancements in SPAD technology include; i) optimized breakdown voltage modelling, ii) reduction of timing jitter through carrier diffusion and electric field uniformity, and iii) improved photon detection efficiency (PDE) through simulation and experimental validation [11].

D. Indirect Time-of-Flight Pixel Development

Indirect time-of-flight (iToF) sensors rely on demodulation performance, which is influenced by factors such as demodulation contrast (DMC), quantum efficiency, and carrier transit time [4]. Optimization strategies include; i) increasing epitaxial layer thickness to enhance light absorption, ii) modifying doping profiles to improve carrier collection, and iii) employing static field transfer pixels with charge-domain operation to enable high-speed demodulation.

E. Global Shutter Technology

Global shutter (GS) sensors address motion artefacts inherent in rolling shutter designs, making them ideal for high-speed imaging applications. Innovations in GS technology include; i) development of charge-domain pixels with higher dynamic range and reduced noise, and ii) 3D stacked GS sensors that integrate dual in-pixel storage with advanced CMOS layers, achieving smaller pixel pitches and improved performance.

F. Meta-Surfaces for Flat Optical Devices

Meta-surfaces, composed of sub-wavelength nanostructures, enable the design of ultra-thin optical devices such as lenses, beam shapers, and spectral filters. These devices rely on precise control of the phase and transmission properties of incident light. The challenge of this technology lies in the materials engineering (to obtain high refractive index contrast), but also in the simulation capabilities and methodology refinement. Indeed, the simulation, but also the visualization tools, are key to design and optimize a large-scale meta-surface optic device.

III. Simulation Tools for Device Optimization

The design and optimization of most (if not all) the CIS technological bricks mentioned above require advanced simulation tools to address the complex interplay between light propagation, carrier transport, and system integration. An ideal simulation framework includes models going from process emulation to atomistic defect description, from 1D transfer matrix to 3D FDTD electromagnetic solvers and from analytic compact models to advanced physical-based semi-classical transport solvers. Moreover a balance between computational efficiency and accuracy is key, especially for multiscale problems. Advanced visualization tools are also mandatory for e.g. simulation output analysis and comparison with measurements. The advent of AI-based simulation is also a game-changer and can move boundaries towards faster and more efficient models for large-scale devices.

A. *Process simulation and Process emulation*

Accurate knowledge of the device's structural geometry is essential for reliable simulation outcomes. Technology computer-aided design (TCAD) process simulation involves physically based modeling of semiconductor fabrication steps such as oxidation, diffusion, ion implantation, etching, and deposition. By simulating these processes, TCAD tools predict the evolution of material profiles, dopant distributions, and interface properties with high spatial resolution. This detailed physical insight enables precise control over device characteristics and performance prediction.

In contrast, process emulation is a modeling approach used to replicate the fabrication steps of semiconductor devices by constructing detailed three-dimensional geometrical heuristic representations of the device structure, emphasizing accurate geometry over detailed process physics. This approach is preferred when detailed physical process simulation is challenging or computationally expensive. This is generally the case for complex and large structures, such as sequential 3D stacking of device layers, as illustrated in Fig. 2. Additionally, capturing realistic geometrical features such as process variations and geometrical line roughness is often challenging to model physically. In such situations, emulated structures, well-calibrated using transmission electron microscopy (TEM) images, can be directly imported into optical solvers, enhancing the fidelity of device geometry representation and improving simulation accuracy [10].

B. *Advanced pixel simulation*

Electromagnetic simulations, such as Finite-Difference Time-Domain (FDTD) and Rigorous Coupled-Wave Analysis (RCWA), are employed to model light interaction with diffractive elements and metal reflectors, enabling detailed analysis of optical phenomena including reflection, diffraction, scattering, and absorption. FDTD provides time-resolved solutions to Maxwell's equations, allowing the study of complex (potentialy non-periodic) large structures, while RCWA efficiently handles smaller periodic structures, such as meta-surface scatterer elements. Together, these methods help optimize device performance by accurately predicting how light propagates through and interacts with complex 3D geometries, which is essential for the design of photonic devices, and advanced sensors as shown in Fig. 3 for a NIR pixel.

To enhance simulation accuracy further and allow comparison with electrical measurement results, as shown in Fig. 4, electrical and optical simulations needs to be coupled. In general, a TCAD drift-diffusion-based device simulation is sufficient to calculate the electrical crosstalk or the efficiency of carrier collection at the electrodes.

However, for high field devices, such as SPADs, traditional TCAD models fail to capture the statistical features of carrier transport. Monte Carlo methods are typically used to provide insights into timing jitter, photon detection efficiency (PDE), and dark current mechanisms [11]. An example of carrier trajectory modelled with MC framework is shown in Fig. 5.

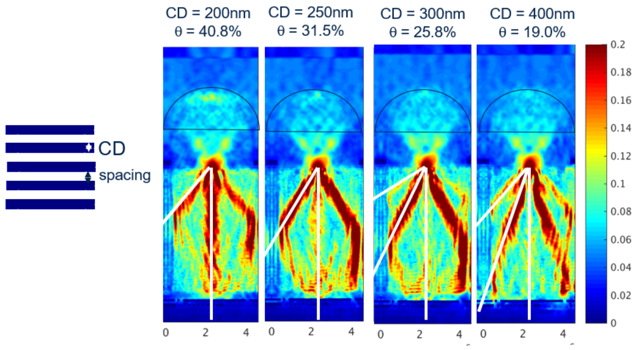

Fig. 3. Light propagation inside a NIR pixel, simulated by FDTD, for diffractive grating with different pitches. The figures shows a 2D cut of a Poynting vector. White lines are showing the position of microlens.

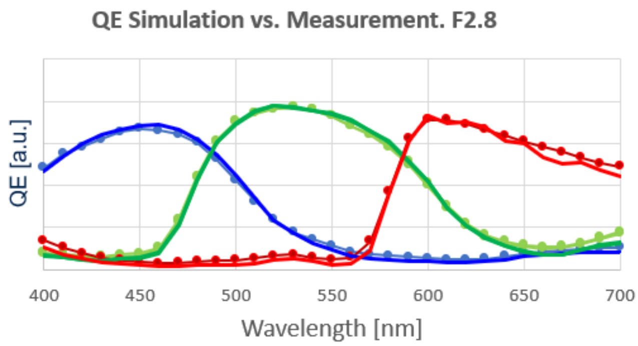

Fig. 4. Comparison of simulated (solid lines) and measured (circle symbols) Quantum Efficiency in a RGB sensor.

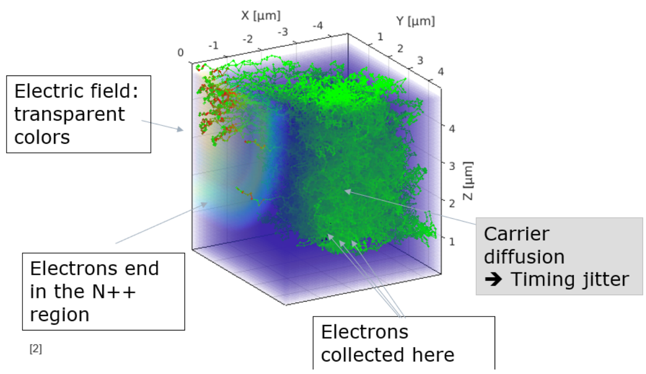

Fig. 5. Particles trajectories in a SPAD device computed with Monte Carlo simulation.

C. *Meta-surface simulation*

The design of meta-surface, composed of sub-wavelength nanoscattered with various sizes and shapes, require the accurate prediction of light propagation through the structure (see Fig. 6).

The near field phase of each pillar is then stitched and propagated. However, traditional simulation methods, such as periodic pillar-wise FDTD, face challenges in accurately modelling the interactions between neighbouring pillars and

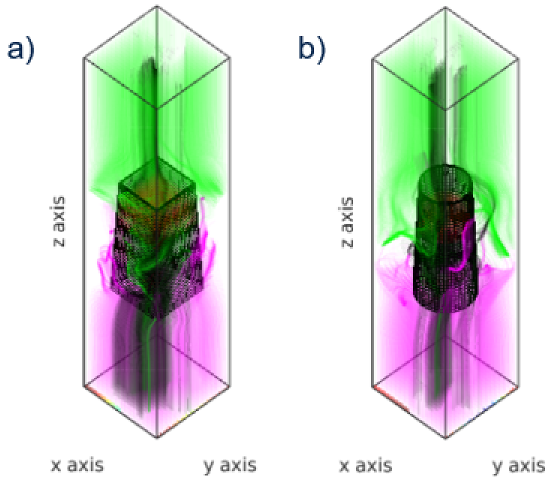

Fig. 6. Field lines across a typical pillar-type metasurface for two different shape: (a) square and (b) round pillar. Crossing lines are highlighted in darker colour, which also superimpose the structure. Non-crossing field lines are highlighted with colour: top to bottom in green and bottom to top in purple.

thus to predict the resulting optical performance.

These challenges prompt the adoption of neural network-based emulation methods. Once trained on electromagnetic solvers, they allow to optimize large-scale diffractive optics, as shown in Fig. 7 [11].

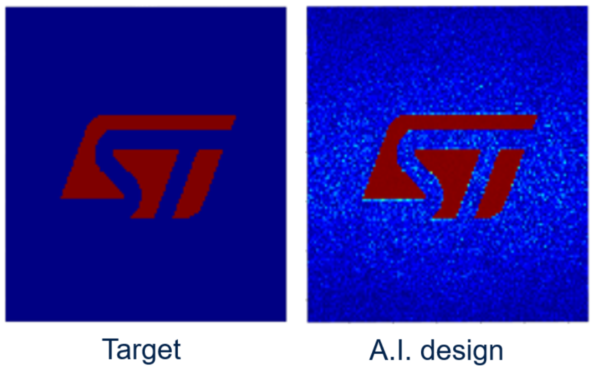

Fig. 7. Metasurface optimization with AI for the an image projection: (left) target and (right) optimization result.

IV. Conclusion

The advancements in 3D stacking and pixel size miniaturization have transformed CMOS image sensor (CIS) design, enabling the development of differentiated pixel architectures tailored to the requirements of emerging applications. Additionally, meta-surface and surface structuration technologies have significantly enhanced the functionality of optical sensors, unlocking new possibilities for high-resolution and energy-efficient imaging solutions.

Sequential 3D stacking and hybrid bonding technologies offer substantial potential for the next generation of optical sensors, fostering breakthroughs in 3D imaging and advanced sensing applications.

Advanced simulation tools can provide competitive advantages during the development phase of optoelectronic devices. Innovative solutions are continuously emerging in the literature, optimizing complex structures in a multiscale and multiphysics approach, with reduced simulation time.

Acknowledgments

The authors acknowledge the contributions of the STMicroelectronics Technologies for Optical Sensor Department and APMS/IMG Division. Special thanks to the co-authors and collaborators for their dedicated research and development efforts.

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