Advances in 3D CMOS image sensors optical modeling: combining realistic morphologies with FDTD

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***Abstract*— This paper describes an innovative methodology to investigate the relationship between device morphology and the optical performance of CMOS image sensors. By coupling a FDTD-based 3D Maxwell solver with silicon-accurate process modeling software, we have been able to analyze the sensitivity of image sensor quantum efficiency with respect to statistical variations in nm-scale device topology. Additionally, we studied pyramidal silicon structuration for quantum efficiency enhancement as proposed in [1].**

Keywords—CMOS image sensor, process modeling, 3D nanophotonic simulation

I. INTRODUCTION

Increasing the quantum efficiency (QE) of high-end CMOS Image Sensors (CIS) is very difficult, due to the impact of dark current on device noise, especially in the near-IR. Nanometer scale variability in device topology can substantially (and unexpectedly) affect both device noise and quantum performance. This impact of pixel stack morphology changes on the optical response of a CMOS sensor can be investigated using 3D FDTD nanophotonic simulation. However, complex 3D shapes built in silicon devices are difficult to model using conventional 3D design modeling tools. In addition, novel pixel structures being developed to increase QE are highly susceptible to degradation of potential gains in light sensing due to uneven surface morphology and emphasize the need for more advanced 3D photonic modeling [1].

II. METHODOLOGY

A. *Process flow modeling*

In this study, we have simulated the optical response of advanced back-side illuminated sensors combining realistic structures emulated with a virtual fabrication platform [2] (Fig. 1) with 3D FDTD simulations [3]. This former 3D voxel-based technology can efficiently account for process-related local (but also statistical) variations of the device morphology (such as edge rounding, interface fluctuations, and non-conformal layer depositions) that can lead to additional parasitic light diffraction and interferences. Our simulation domain consisted of a 2x2 pixel architecture in a Bayer pattern. The process flow is integrally described within the modeling tool in a step-by-step manner, from Deep Trench Isolation (DTI) and Shallow Trench Isolation (STI) to back-side thinning. We note that accurate process modeling requires a rigorous calibration procedure. Nonetheless, as shown in Fig. 2, the simulated structure can accurately reproduce TEM cross sections, including roughness, irregularities and distortions.

B. *Samples description*

We executed a Delaunay meshing algorithm [4] after building the final 3D structure (Fig. 3a). This meshing

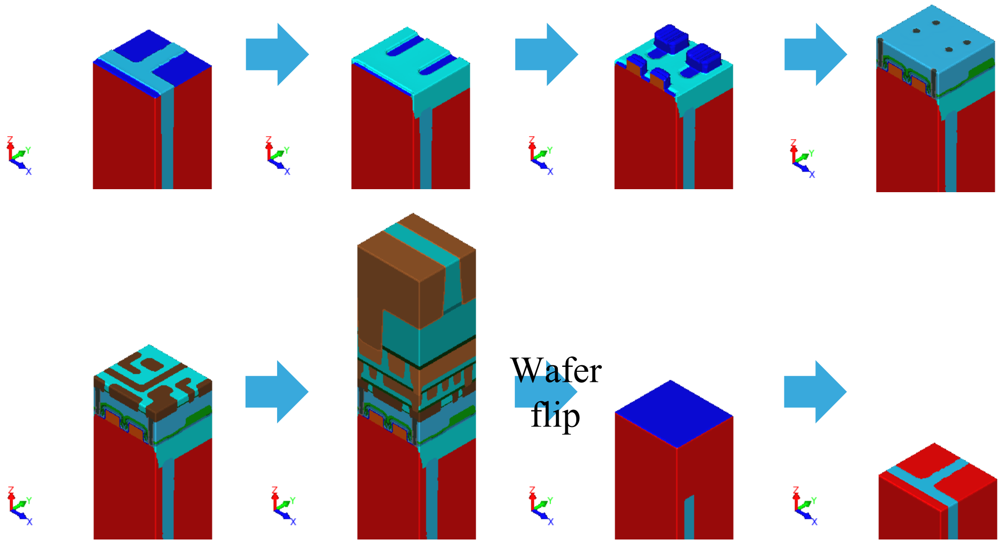

Fig. 1 3D process flow modeling of test case.

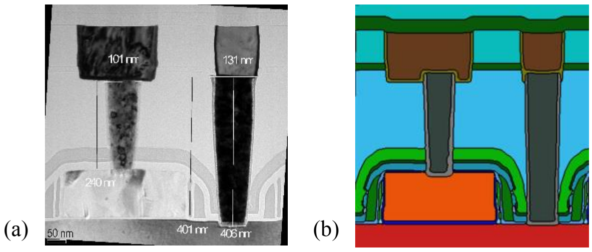

Fig. 2 (a) TEM cross section in FEOL and (b) corresponding 3D structure emulated in SEMulator3D®.

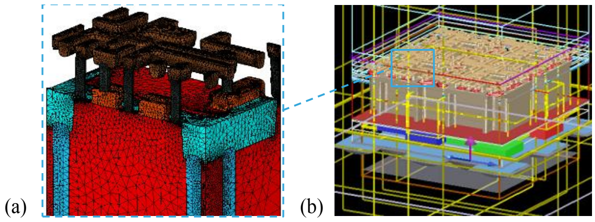

Fig. 3 (a) Magnified view of mesh structure of CIS devices and (b) its integration within the optical solver (substrate and dielectrics not shown).

algorithm consists of two main steps: a pre-processing step that extracts multi-material interfaces from the 3D voxel model, and the Delaunay mesh step that directly creates triangular surface and tetrahedral mesh elements that match the extracted surfaces. The topology of key devices e.g. DTI, STI, CMOS polysilicon gates and first level of Cu-interconnections (Metal1 or M1) are then imported into the optical design modeling tool as STL files (Fig. 3b), generated by the meshing.

Ideal pixel topology, which relies on building all devices from extrusion of GDS mask layers, is used as the reference model, as shown in Sample A (Fig. 4a). The same structure with fine grain topology, based upon the mesh import, is displayed in Fig. 4b and shown in Sample B. The latter will be compared to the reference case in the following section. Sample C is identical to sample B except that voids are voluntarily introduced in the vicinity of DTI. Indeed, although depending upon the DTI process used, the filling of high aspect ratio trenches with oxide can induce the formation of voids in the vicinity of the trenches. This voids, which size does not exceed 40nm in width, are emulated using non-conformal deposition model (Fig. 4c). Finally, this methodology has been extended to evaluate design and process options to increase the QE. One solution consists of structuring the back-side surface of the Si substrate to increase the optical path for light in the photodiode [1,5]. To do so, a KOH-based chemistry is emulated to reproduce pyramidal patterns, as depicted in Sample D (Fig. 4d).

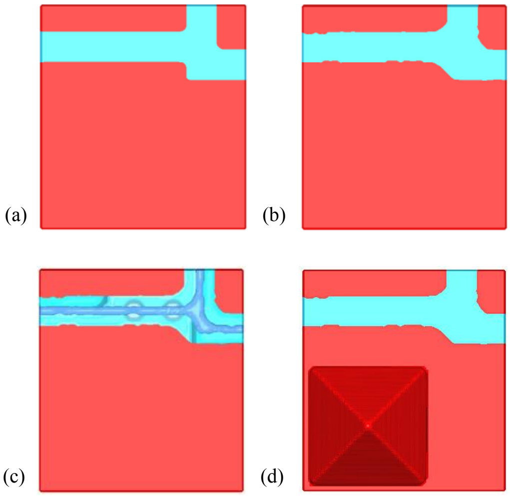

Fig. 4 Process emulation of a region of interest, viewed from the back side with (a) an ideal topology with planar Si surface (Sample A), (b) a realistic topology with planar Si surface (Sample B), (c) a realistic topology with planar Si surface and voids inside DTI (Sample C, filling oxide being transparent for clarity purpose), and (d) a realistic topology with structured Si surface (Sample D). Light blue color represents the DTI oxide and red color the Si active area. The pyramidal structure can be seen in (d).

III. OPTICAL SIMULATION RESULTS

Unless specified, identical simulation conditions are set for the samples described in the previous section. 3D electromagnetic FDTD method is ran using a monochromatic collimated source from 400nm to 1000nm with steps of 20nm. Light is set with an incidence angle of 0° and two orthogonal polarizations are averaged incoherently to reproduce unpolarized light. Finally, Bloch boundaries conditions are applied and the maximum mesh step settings are 20nm in z and uniform at 10nm in x/y.

A. Sensitivity on QE between ideal and realistic topologies

The optical responses of an ideal pixel structure (Sample A) and a realistic pixel structure (Sample B) are shown in Fig. 5. Minor topological changes to an ideal CIS structure can generate a small percentage variation in absorption for red and NIR wavelengths. The transmission above M1 is particularly sensitive to topology changes for wavelengths greater than 600nm. This drift is well correlated with the differences of absorption in M1 layer (Fig. 6), emphasizing that the etch profile of metal interconnections and corner rounding play a non-negligible role in light absorption in the whole pixel. Discrepancies between ideal and realistic structures are clearly evidenced in cross sections of light propagation in two pixels at 920nm (Fig. 7). Therefore, the absorption in metal lines is critical and must be accurately simulated as less absorption in metal lines will lead

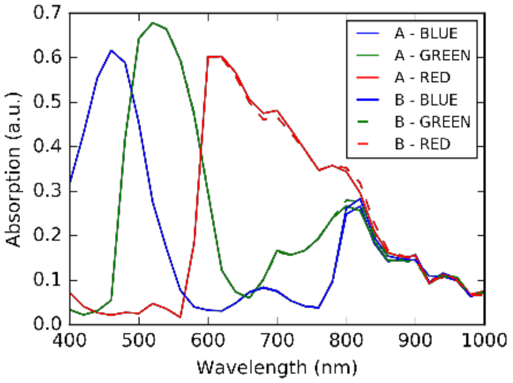

Fig. 5 FDTD simulations of light absorption in blue, green and red pixels in an ideal structure (Sample A in solid line) and in a realistic structure with expected manufacturing variability (Sample B in dashed line).

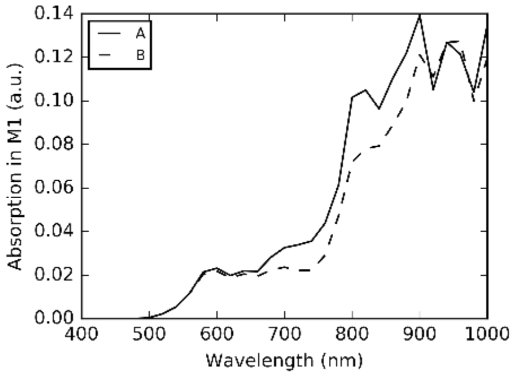

Fig. 6 Absorption of light in the first layer of metal interconnections in an ideal structure (Sample A in solid line) and in a realistic structure with expected manufacturing variability (Sample B in dashed line).

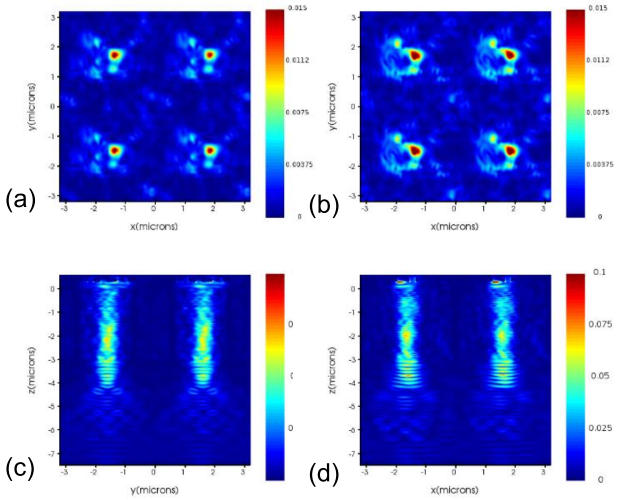

Fig.. 7 Comparison of light propagation simulated in two pixels: XY cross-sections above M1 between ideal (a) and realistic structure (b), YZ cross-sections between ideal (c) and realistic structure (d).

to more reflections back to the photodiode, i.e. more QE in the pixel.

B. *Sensitivity on QE between structure with filled DTI and structures with voids inside DTI*

The presence of voids in oxide filling DTI and their impact on optical performances are investigated in Sample B. In this case, incidence angle is set at 10° to force the light to go through the DTI. We discovered that 40 nm wide voids do not significantly affect the optical performance of a pixel (Fig. 8). This result highlights the minimal impact of void defects, which should in principle depend on the statistical occurrence of voids as well as their average size.

C. *Sensitivity on QE between structure with planar back-side Si surface and structured back-side Si surface*

QE enhancement solution with back-side silicon surface texturing is evaluated with Sample D. Process simulations are coupled with design variations of inverted pyramids pitch and size. Optical simulations show a x1.6 gain in absorption at 940nm for an optimal geometry consisting of a 3x3 array of pyramids with a square base of 400nm and a spacing of 100nm between each pyramid. This is compared to the reference case, Sample B, with a planar back-side surface (Fig. 9).

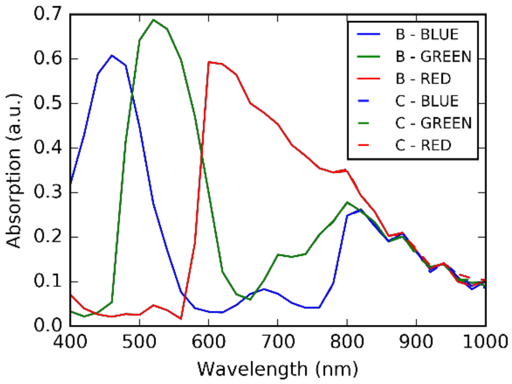

Fig. 8 FDTD simulations of light absorption in blue, green and red pixels in a realistic structure with perfectly filled DTI (Sample B in solid line) and in a realistic structure with 40nm wide voids inside DTI (Sample C in dashed line) at 10° incidence angle.

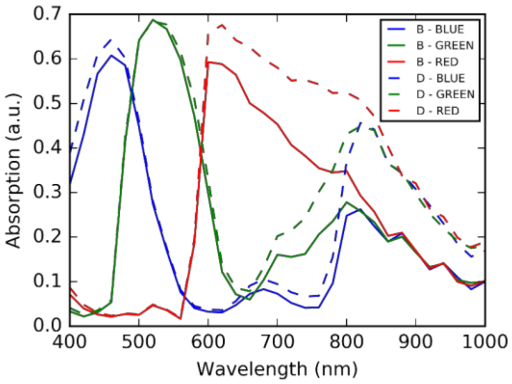

Fig. 9 FDTD simulations of light absorption in blue, green and red pixels in a realistic structure with planar back-side surface (sample B in solid line) and in the same structure with a 3x3 array of inverted pyramids (sample D in dashed line).

IV. CONCLUSIONS

Coupling a FDTD-based 3D Maxwell solver and a 3D virtual fabrication platform, using well calibrated process modeling of CIS, enables understanding of process variations effects which are not taken into account in conventional photonic modeling. This paper demonstrates the need to have an accurate morphological description of metallic interconnections since they play a major role in the absorption of light at pixel level, hence in the estimated QE. Moreover, the methodology used in this paper is particularly well-adapted for studying novel architectures using new Si structuration solutions to improve the optical performance of next generation CIS.

Full interoperability of the process modeling tool and 3D FDTD nanophotonic simulation will enable new and advanced studies. For example, the resilience of the quantum efficiency gain with respect to process variations (such as lithography misalignment, corner rounding of pyramidal patterns, as well as conformality of passivation layers deposited in etched cavities) will be characterized.

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