

Quantum Efficiency Simulation Using Transport Equations

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Abstract - Quantum efficiency is an important image sensor characteristic, connected to the wavelength-dependent signal collection and crosstalk. Simulation of quantum efficiency provides insight into the physical mechanisms within the pixel to guide development. We present a method of obtaining a numerical, physically-based photodiode model which can be used for faster predictions of QE, as well as provide graphical insight into the processes of crosstalk. Simulations are compared against experimental results for a $1.1\mu\text{m}$ BSI pixel.

INTRODUCTION

As pixel dimensions shrink, the need for accurate modeling increases, in order to better understand and minimize the effects optical and electrical crosstalk. Once good correlation between simulation and experiment has been established the simulation can be explored to understand the physical mechanisms.

Simulation of quantum efficiency comprises three parts: (1) optical excitation, modeled as electromagnetic plane waves interacting with the interconnect layers and silicon device structure; (2) absorption in the silicon to create photocarriers; and (3) transport of the photocarriers into the photodiode potential well through drift and diffusion.

Simulation can be accomplished inside an integrated environment, consisting of an electromagnetic solver and a TCAD device simulator. In this method a solution which iterates between the device and the EM solver is required for each wavelength. This must be repeated for each variation in either structure or illumination condition.

The alternative is to separate the problem into optical and device simulations, each using a tool suited to its purpose, with the final solution being a matrix convolution. Our approach uses a commercial TCAD suite of process and device solvers, a commercial FDTD (finite-difference time-domain) optical solver, and Aptina-developed software using the Comsol platform for generation of the photodiode model.

OPTICAL GENERATION

Electromagnetic fields are solved using the FDTD method. This provides broadband steady-state

electric and magnetic fields via Fourier transform. We consider a summation of individual plane wave simulations in linear superposition to model the response of the camera aperture. In particular, we model an f/2.8 aperture where the where incidence angles range from 0° to 10° .

Figure 1 shows the 3d layout of a BSI (backside illuminated) pixel, which includes micro-lens and color filter arrays on top of an anti-reflective coating at the silicon backside interface. The front surface of silicon abuts to silicon-dioxide. We exclude any frontside structure from our simulation, terminating the simulation domain in oxide with a perfectly matched layer, so that there are no reflections beyond the silicon-oxide interface. The lateral boundary conditions are periodic, so that an infinite array of pixels is modeled.

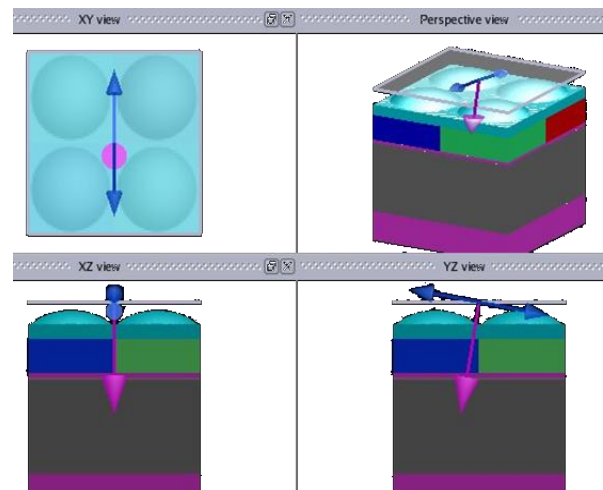


Figure 1 - 3d pixel layout for FDTD simulation. Illumination source is shown at 10° incidence

Quantum efficiency at a particular wavelength is calculated as the ratio of the power dissipated in a region of silicon to the input power. This method of computing QE is fast once the FDTD simulation has completed and Fourier transforms have been calculated.

Figure 2 shows the electrostatic potential obtained from TCAD simulation for a $2.0\mu\text{m}$ thick BSI silicon region of a 3×3 block of pixels. A rectangular box can be drawn which correlates with the strong electric field region of the center pixel's photodiode. This is a useful approximation: inside the box all photocharge is collected due to high drift field, and outside diffusion plays an increasingly important role.

More boxes may be added to the model, outside the main box, with different weighting factors, as shown

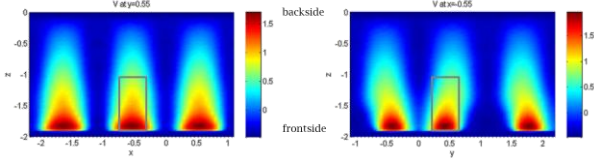


Figure 2 – 2d vertical x- and y-cuts of pixel in silicon region showing electrostatic potential

in figure 3. The weighting factors are given for the center photodiode. The 100% collection region for one photodiode is a 0% collection region for all other photodiodes. Photocollection must eventually drop to zero away from the central region.

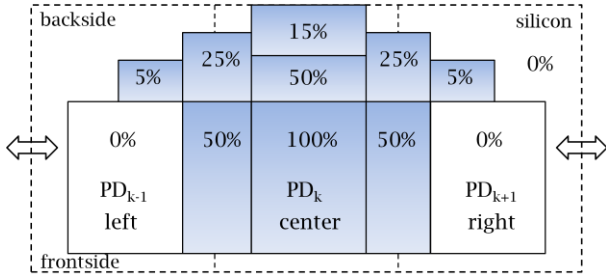


Figure 3 – 3 pixel cross-section showing additional collection of center pixel, as shown by the shaded regions

Taking the limit in which the number of individual boxes increases while their size decreases results in a continuous photodiode collection probability model. In this case QE is determined as the integral of optical generation times some weighting function,

$$(1) \quad S_k = \int_{Si} W(\mathbf{x}) G_\lambda(\mathbf{x}) d\mathbf{x}$$

where S_k is the signal collected by pixel k , \mathbf{x} is a point in space, W is the weighting function, and G_λ is the steady-state optical generation at a particular wavelength. We integrate over the entire silicon region, but in practice we need only integrate over the region of silicon in which W is non-zero. We obtain the signal for pixel k , which in a Bayer pattern is representative of all other pixels sharing the same color filter, photodiode layout, and approximate location within the pixel array.

We determine the weighting function by breaking the signal into two components: the interior of a closed surface inside the high-field region, denoted PD_k , and the exterior region. The size and shape of this region is not critical, but it must lie within the drift-dominated region. Inside PD_k the weighting function W has value of 1.0. Outside of PD_k we must determine W . We can express pixel signal as

$$(2) \quad S_k = S_k^{int} + S_k^{ext} = \int_{<PD_k} G_\lambda(\mathbf{x}) d\mathbf{x} + \int_{>PD_k} W(\mathbf{x}) G_\lambda(\mathbf{x}) d\mathbf{x}$$

We evaluate the 2nd integral to formulate an expression for W by considering the following equivalence, namely, that the pixel signal is equal to the sum all photocharge generated within PD_k plus the total photocurrent which flows into PD_k . The current flowing into PD_k , i.e. the 2nd term in (2), can be expressed as:

$$(3) \quad S_k^{ext} = \int_{PD_k} \mathbf{J}(\mathbf{x}) \cdot \mathbf{n} d\sigma$$

which is the normal component of the photocurrent density integrated on the closed surface PD_k . We now seek an expression for the current density.

CHARGE TRANSPORT MODEL

We model transport of free carriers in a semiconductor with the continuity equation

$$(4) \quad \frac{du(\mathbf{x},t)}{dt} = \frac{1}{q} \nabla \cdot \mathbf{J}(\mathbf{x}) + G_\lambda(\mathbf{x})$$

where u is the electron concentration, q is the electron charge, and \mathbf{J} is the electron current density, which is the sum of diffusion and drift components. In steady-state the left side of (4) is zero.

The flux operator Φ is defined as

$$(5) \quad \Phi u(\mathbf{x}) \equiv \mathbf{J}(\mathbf{x}) = qD\nabla u(\mathbf{x}) + q\mathbf{v}(\mathbf{x})u(\mathbf{x})$$

Here D is the diffusion coefficient for electrons, \mathbf{v} is the electron drift velocity, equal to the product of electron mobility and \mathbf{E} , the (static) electric field. We consider the electric field to be essentially constant during of the pixel integration time period, and that it dominates the optical field. We do not consider thermal generation and recombination.

Combining the continuity and current density equations we obtain the steady-state transport equation for electrons:

$$(6) \quad \mathcal{A}u(\mathbf{x}) \equiv -\nabla \cdot (D\nabla u(\mathbf{x}) + \mathbf{v}(\mathbf{x})u(\mathbf{x})) = G_\lambda(\mathbf{x})$$

which defines the transport operator \mathcal{A} .

Instead of solving the transport equation directly for a particular optical generation, we solve the following:

$$(7) \quad \mathcal{A}G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y})$$

where $\delta(\mathbf{x} - \mathbf{y})$ is the Dirac-delta function, and $G(\mathbf{x}, \mathbf{y})$ is the Green's function for the operator \mathcal{A} . This describes a response at \mathbf{x} to a point source at \mathbf{y} .

It can be shown that the solution for electron concentration, u , is given as

$$(8) \quad u(\mathbf{x}) = \int_{Si} G(\mathbf{x}, \mathbf{y}) G_\lambda(\mathbf{y}) d\mathbf{y}$$

Thus the solution for the carrier concentration is found as the convolution of the Green's function and the optical generation. Having obtained an expression for the carrier concentration in (8) we can obtain \mathbf{J} by applying Φ_x (denoting action on the x-coordinate) in (3). After rearranging the order of integration and differentiation we find

$$(9) \quad S_k^{ext} = \int_{S_i} (\int_{PD_k} \Phi_x \mathcal{G}(\mathbf{x}, \mathbf{y}) \cdot \mathbf{n} d\sigma) G(\mathbf{y}) d\mathbf{y}$$

We identify the weighting function W as the integral of the flux of the Greens' function

$$(10) \quad W(\mathbf{x}) = \int_{PD_k} \Phi_x \mathcal{G}(\mathbf{x}, \mathbf{y}) \cdot \mathbf{n} d\sigma$$

Thus our problem becomes finding the solution to (7) for a particular electric field. In practice we find the solution to (10) as well, by integrating the flux of the Green's function, stepping the point source throughout the silicon region. Here W extends to a 3x3 cell of pixels because it becomes sufficiently close to zero at a distance of one pixel beyond the central pixel.

The Green's function accounts for drift and diffusion; the optically generated photocurrent can be considered to be a weighted sum of point sources. We refer to it as the photodiode collection probability.

RESULTS

We have implemented this procedure as an application of the finite element method commercial software Comsol.

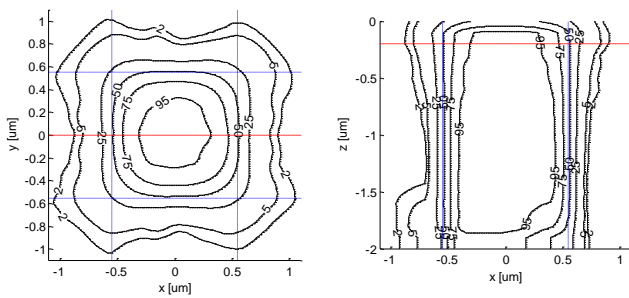


Figure 4 – 2d horizontal and vertical cuts of pixel illustrating photodiode collection probability. The blue dashes indicate pixel boundaries and the red dashes indicate cross-section cut lines.

Figures 5 and 6 show 2d cross-sections of the 3d optical generation overlaid with the photodiode collection at a wavelength of 550nm. The periodic 2x2 pixel array has been extended to a 3x3 cell with the red pixel placed at the center. The procedure is repeated by translating the optical generation to obtain the response of the other pixels in the 2x2 cell, and at other wavelengths.

Figure 7 shows the product of optical generation and the photodiode weighting function, which reveals the signal density. This distribution is then integrated numerically to obtain the QE signal for the red pixel at a wavelength of 550nm. Figure 8 shows the crosstalk components.

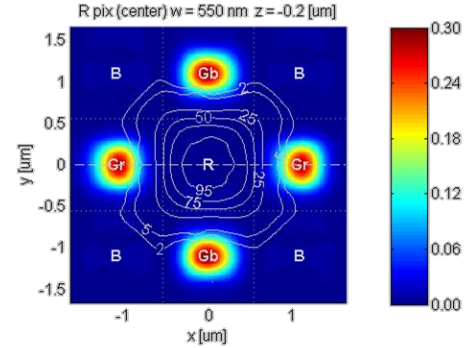


Figure 5 – 2d horizontal cut of optical generation (color) and photodiode collection probability (contour lines)

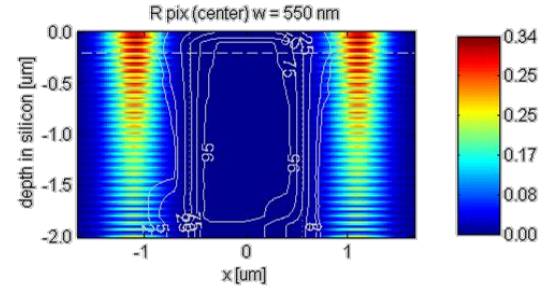


Figure 6 – 2d vertical cut of optical generation (color) and photodiode collection probability (contour lines)

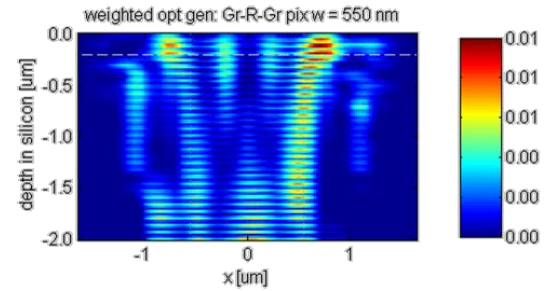


Figure 7 - Optical generation multiplied by collection probability weighting function

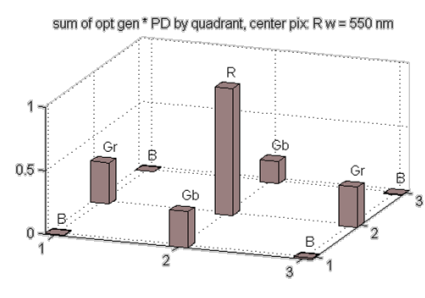


Figure 8 - Relative signal collected from each pixel in 3x3 cell illuminated at normal incidence

Repeating this process for each pixel across the visible wavelength band results in QE at 0°

incidence, as shown in figure 9. We display the central pixel signal and crosstalk components for the red pixel.

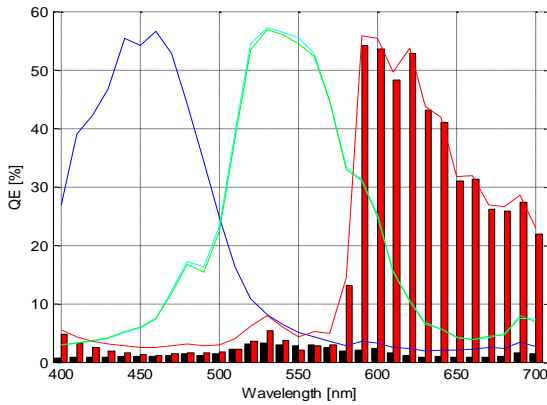


Figure 9 – Simulated QE at 0° incidence. The bars show primary (red) and secondary (black) signal contributors for the red pixel.

At 10° incidence we see that the optical beam has encroached significantly into the central photodiode collection region. Figure 10 shows how the beam begins to shift into the neighboring pixel. Photo signal is dominated by overlap of the beam with the neighboring collection region.

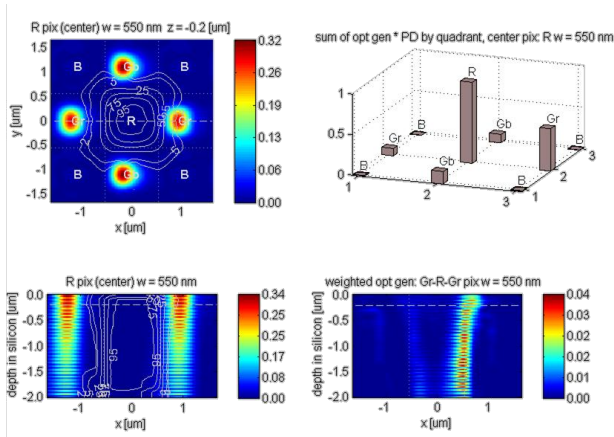


Figure 10 – Optical generation and photodiode collection contours for 10° incidence

Combining the response at 0° and 10° (for several additional azimuth angles) we obtain QE for an f/2.8 aperture. The comparison of the simulation prediction and experiment in Figure 11 shows agreement in peak QE and in the crosstalk. Residual differences are an opportunity for further refinement including the precision of the physical and material properties assumed in the simulation (e.g., CFA transmission and thickness).

CONCLUSION

A novel photodiode model based on the method of Green's functions is presented. The steady-state optical generation is point-wise multiplied by the PD

model, which acts as a weighting function. The weighted sum is integrated to obtain the pixel signal

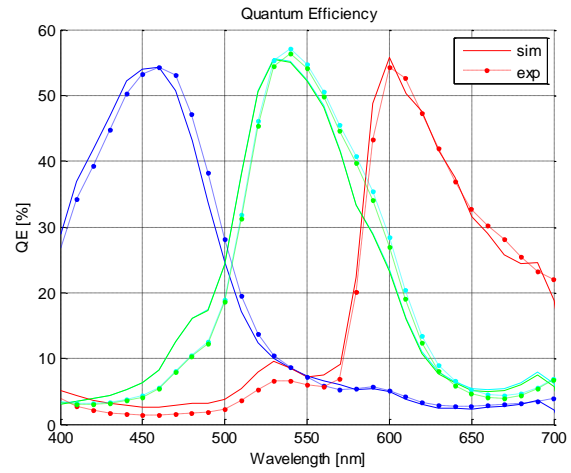


Figure 11 – Simulated QE compared with experimental measurement for 1.1 μm BSI pixel for f/2.8 aperture.

for a given optical condition. The extension of the collection probability into a neighboring pixel's geometry graphically illustrates the effect of the diffusion component of charge transport.

We can identify factors which affect collection performance, including backside collection capability and lateral collection spreading (determined by the backside field strength and conditions at the back surface). The lateral extent of the photocollection region near the front surface is important for isolation for the case of 10° incidence. Design of the pixel can be improved by understanding the individual effects, such as spread of the optical beam and its interaction with the photodiode collection. A small collection probability on the order of 1-2% has a large impact on crosstalk when it extends into regions of the neighboring pixel which have a high optical generation rate.

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