3D Simulation of PDE and Jitter in SPAD Devices.

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Abstract

In this paper we present a full 3D simulation methodology to extract Photon Detection Probability (PDP) and Jitter of Single-Photon Avalanche Diode (SPAD) Devices. The simulation results are compared with measurements on devices and show good agreement with the experiments.

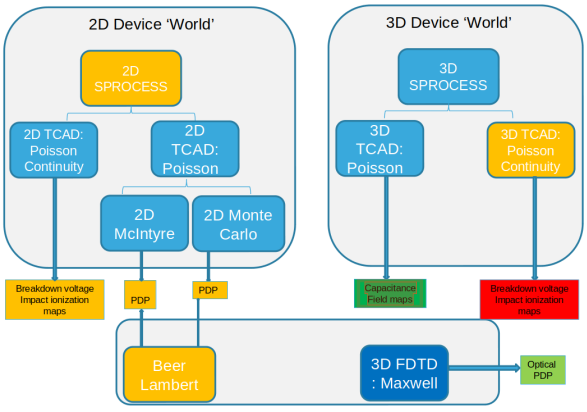
Keywords— single-photon avalanche diode (SPAD), photon detection probability (PDP), jitter, avalanche breakdown probability, breakdown voltage

1 Introduction

Single-photon avalanche diodes (SPADs) are key opto-electronics devices.

2 Device structure and TCAD simulation

Figure 1: SPAD simulation workflow



3 Avalanche breakdown probability

The avalanche breakdown probability is computed by the means of the well known McIntyre model [Oldham et al., 1972]. We briefly recall the model derivation : Let $P_e(x)$ be the probability that an electron starting at x in the depletion layer triggers an avalanche and $P_h(x)$ the same probability for an hole starting at x. Straightforwardly, the probability that neither an hole nor an electron starting at x trigger an avalanche is given by $(1-P_e(x))(1-P_h(x))$. Thus, the probability that either the hole or the electron trigger an avalanche, noted P_{pair} is :

$$\begin{aligned} P_{pair}(x) &= 1-(1-P_e(x))\,(1-P_h(x)) \\ &= P_e + P_h - P_e P_h \end{aligned}$$

Now, the probability that an electron starting at $x+dx$ triggers an avalanche is : The probability that the electron reaches the position x and triggers an avalanche in x plus the probability that it triggers an avalanche between x and $x+dx$ less the probability of the intersection of the two previous events. It writes :

$$\begin{aligned} P_e(x+dx) &= P_e(x) + \alpha_e(x)dxP_{pair}(x) - P_e(x)\alpha_e dxP_{pair}(x) \\ &= P_e(x) + \alpha_e(x)dx(P_e(x)+P_h(x)-P_e(x)P_h(x)) \\ &\quad - P_e(x)\alpha_e(x)dx(P_e(x)+P_h(x)-P_e(x)P_h(x)) \\ &= P_e(x) + dx\,\alpha_e(x)(P_e(x)+P_h(x)-P_e(x)P_h(x))(1-P_e(x)) \end{aligned}$$

Where α_e is the electron linear ionization rate : the probability by length that an electron create an impact ionization event.
One can rearrange the terms to obtain :

$$\frac{P_e(x+dx)-P_e(x)}{dx} = \alpha_e(x)(P_e(x)+P_h(x)-P_e(x)P_h(x))(1-P_e(x))$$

Which leads to the first ordinary differential equation :

$$\frac{dP_e}{dx} = (1-P_e)\alpha_e(P_e+P_h-P_eP_h)$$

The same reasoning applies to the probability that an hole starting at $x-dx$ triggers an avalanche. Which leads to the second ordinary differential equation :

$$\frac{dP_h}{dx} = -(1-P_h)\alpha_h(P_e+P_h-P_eP_h)$$

Therefore we can draw up the McIntyre system :

$$\begin{cases} \dfrac{dP_e}{dx} = (1-P_e)\alpha_e(P_e+P_h-P_eP_h) & (1) \\ \dfrac{dP_h}{dx} = -(1-P_h)\alpha_h(P_e+P_h-P_eP_h) & (2) \end{cases}$$

for $0 \le x \le W$.
Adding the couple of boundary value conditions :

$$\begin{cases} P_e(x=0) = 0 & (3) \\ P_h(x=W) = 0 & (4) \end{cases}$$

we have a full 1D coupled and non-linear boundary value problem. Since we have to extract this value at a large number of points, we use a self-made solver, embedded in a C++ program. This solver uses finite difference method coupled with a Newton's method to care of the non-linearity of the problem [Ascher et al., 1987]. The algorithm is different from those implemented in MatLab routine (bvp4c) or SciPy function (solve_bvp) [Kierzenka and Shampine, 2001] but the comparison with these tools show no difference.
We set the following notations :

$$Y(x) = \begin{pmatrix} P_e(x) \\ P_h(x) \end{pmatrix}$$

$$f(Y,x) = \begin{pmatrix} (1-Y_1(x))\alpha_e(Y_1(x)+Y_2(x)-Y_1(x)Y_2(x)) \\ -(1-Y_2(x))\alpha_h(Y_1(x)+Y_2(x)-Y_1(x)Y_2(x)) \end{pmatrix}$$

$$g(s_1,s_2) = \begin{pmatrix} s_1 \\ s_2 \end{pmatrix}$$

The problem hence reads :

$$\begin{cases} Y'(x) = f(Y,x) & (5) \\ g(Y(0),Y(w)) = 0 & (6) \end{cases}$$

3.1 Newton scheme

3.1.1 Finite differences approximation

Let $\mathscr{M}$ be the mesh on which we work. It is given by the streamlines construction. So we have :

$$\mathscr{M} : 0 = x_1 < x_2 < x_3 < \cdots < x_N < x_{N+1} = w$$

The approximated solution on mesh $\mathscr{M}$ is $Y_{\mathscr{M}} = (y_1, y_2, \cdots, y_N, y_{N+1})$, where y_i is the approximation of $Y(x_i)$.
For numerical approximation we again consider the mesh $\mathscr{M}$ and denote the vector of approximate solution values at mesh points by $Y_{\mathscr{M}}$. The trapezoidal scheme of finite difference methods is given by :

$$\frac{y_{i+1}-y_i}{h_i} = \frac{1}{2}\left(f\left(x_{i+1},y_{i+1}\right)+f\left(x_i,y_i\right)\right) \quad 1 \le i \le N \qquad (7)$$

$$g\left(y_1,y_{N+1}\right) = 0 \qquad (8)$$

Thus we obtain a system of $2(N+1)$ algebraic equations for the $2(N+1)$ unknowns $Y_{\mathscr{M}}$. Unlike before, though, these equations are non-linear. The number N depends on the precision we take when we construct the streamlines. We commonly take a range of $[1nm, 10nm]$, we then have $N \sim 5000$. Fortunately, the Jacobian matrix of this system is rather sparse, as we shall see below.

3.1.2 Newton method

We consider a system of equation written in the compact form :

$$\mathbf{F(s) = 0}$$

We define a function $\mathbf{G}$:

$$\mathbf{G(s)} = \mathbf{s} - \left[\mathbf{F}'(\mathbf{s})\right]^{-1}\mathbf{F(s)}$$

with $\mathbf{F}'(\mathbf{s})^{-1}$ the inverse of the Jacobian matrix of F :

$$\mathbf{F}'(\mathbf{s}) = \frac{\partial \mathbf{F(s)}}{\partial \mathbf{s}}$$

Then the newton method iterative method is given by the iteration :

$$\mathbf{s}^{k+1} = \mathbf{G}(\mathbf{s}^k)$$

So the algorithm will first solve the linear system :

$$\mathbf{F}'\left(\mathbf{s}^k\right)\boldsymbol{\xi} = -\mathbf{F}\left(\mathbf{s}^k\right) \qquad (9)$$

And then simply do :

$$\mathbf{s}^{k+1} = \mathbf{s}^k + \boldsymbol{\xi} \qquad (10)$$

3.1.3 Construction of the linear system

Let $\mathbf{N}_{\mathscr{M}}$ be the following discrete differential operator :

$$\mathbf{N}_{\mathscr{M}}\mathbf{y}_i = \frac{y_{i+1}-y_i}{h_i} - \frac{1}{2}\left(f\left(x_{i+1},y_{i+1}\right)+f\left(x_i,y_i\right)\right)$$

Then

$$\mathbf{F(s)} = \begin{pmatrix} N_{\mathscr{M}}\mathbf{y}_1 \\ N_{\mathscr{M}}\mathbf{y}_1 \\ \vdots \\ N_{\mathscr{M}}\mathbf{y}_N \\ g(y_1,y_{N+1}) \end{pmatrix}$$

We set

$$\boldsymbol{\xi} = \begin{pmatrix} \mathbf{w}_1 \\ \mathbf{w}_2 \\ \vdots \\ \mathbf{w}_N \\ \mathbf{w}_{N+1} \end{pmatrix}$$

So that the Newton method iteration becomes :

$$\frac{\mathbf{w}_{i+1}-\mathbf{w}_i}{h_i} - \frac{1}{2}\left[A(x_{i+1})\mathbf{w}_{i+1} + A(x_i)\mathbf{w}_i\right] = -\mathbf{N}_{\mathscr{M}}\mathbf{y}_i^k \quad 1 \le i \le N \qquad (11)$$

$$B_a w_1 + B_b w_{N+1} = -g\left(y_1^m, y_{N+1}^m\right) \qquad (12)$$

Where A is the following matrix :

$$A\left(x_j\right) := \frac{\partial f}{\partial y}\left(x_j, \mathbf{y}_j^k\right)$$

And with

$$B_a = \frac{\partial g(\mathbf{y_1^k}, \mathbf{y_{N+1}^k})}{\partial \mathbf{u}}, \quad B_b = \frac{\partial \mathbf{g}(\mathbf{y_1^k}, \mathbf{y_{N+1}^k})}{\partial \mathbf{v}}$$

which here turns into :

$$B_a = 1, \quad B_b = 1$$

3.1.4 Final algorithm and comparison with SciPy function

The corresponding algorithm is details at algorithm 1. The algorithm results were checked with the SciPy routine as a reference. When the number of points is greater than 500, the relative error is always bellow 1%.

Figure 2: Comparison of the Newton's method agaisnt the SciPy routine with 512 points.

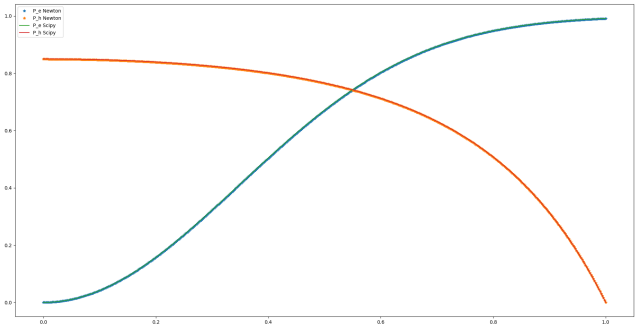
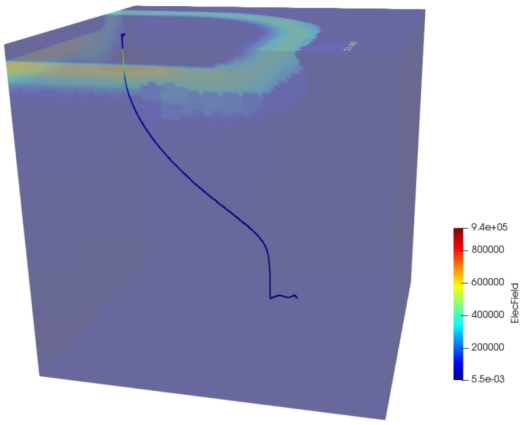


Figure 3: Field line of electric field inside the device



4 Jitter modeling

5 Results and comparisons with experiments

6 Discussion

Algorithm 1: Newton's Method Solver for BVP

input : The Boundary value Problem
input : The Mesh $\mathcal{M}$
input : An initial guess of $Y_{\mathcal{M}}$
input : A maximal tolerance TOL
input : A maximal number of iterations
output: The Solution $Y_{\mathcal{M}}$
output: The final residual error

RES $\leftarrow$ 1000 ;
$NbIterations \leftarrow 0$;
Initialize $w_{\mathcal{M}}$ as a vector of size 2N;

while $RES > TOL$ *and* $NbIterations <$ $MaxNbIterations$ **do**
  for i=1 *to* 2N **do**
    Construct S_i;
    Construct R_i;
    Construct $q_i = -\mathbf{N}_{\mathcal{M}} y_i$;
  Construct A;
  Construct β;
  Solve $Aw_{\mathcal{M}} = \hat{\beta}$;
  for i=1 *to* 2N **do**
    $y_i \leftarrow y_i + (w_{\mathcal{M}})_i$
  $RES \leftarrow ||w_{\mathcal{M}}||$;
  $NbIterations \leftarrow NbIterations + 1$;
if $RES \leq TOL$ **then**
  //The method has converged ;
  return Y;
else
  //The method has converged ;
  return Error : No Convergence

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