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A Numerical Simulation and Modeling of Poisson Equation for Solar Cell in 2 Dimensions

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Abstract. Solar energy is one of the primary sources of energy replacing fossil fuels due to its abundance. Its versatility and environmental friendliness has made it one of the most promising renewable sources of energy. Solar cells convert solar energy into Electrical Energy. The effort to improve the efficiency of these cells and the reduction of their costs has been a major concern for a long time. Modeling of various structures of solar cells provides an insight into the physics involved in its operation and better understanding of the ways to improve their efficiency. This work modeled Poisson Equation in 2D for an abrupt and linearly graded charge densities system with arbitrary points in space. Linear approximation and differentials, finite difference method, boundary conditions and MATLAB were used to obtain the solution. This is the first step in developing a general purpose semiconductor device simulator that is functional and modular in nature. It was observed that highest electric potential was obtained where the point charge was placed for linearly graded and doping type changed over a small distance compared to the extent of the depletion region for abrupt p-n junction. By solving Poisson equation, voltage, electric field, electric charge density and density of free carriers inside the solar cell can be known.

1. INTRODUCTION

It is no news that there is a looming energy crisis due to the fact that the world reserve of fossil fuels is limited. But renewable energies can potentially replace the energy from fossil fuel and mitigate the crisis. The sun illuminates our planet and supplies it by more than 800 times the global current energy consumption [1]. Light energy from the sun which is a renewable energy can be harnessed by the use of photovoltaic cells also called solar cells to give electricity but with varying degrees of efficiencies. There is a need to optimize the efficiencies of these solar cells prior to fabrication and mass production [2]. This is where device simulation and modeling come in [2]. Solar cell can actually be described by Semiconductor equations [3]. These equations describe the behavior of charge carriers under the influence of an electric field or light in the case of solar cells. One of these equations is the Poisson equation, as this equation relates the voltage gradient of space charge density [4]. Also to provide a tool that can supplement solar cell modeling, semiconductor physics and to construct basic solar cell device equation using MATLAB, Poisson equation needs to be solved numerically, with arbitrary point in space for flexibility purpose. The Poisson equation is a very powerful tool for modeling the behavior of electrostatic systems, but unfortunately can only be solved analytically for very simplified models [5]. As a result of this, numerical simulation must be carried out in order to model the behavior of complex geometries with practical value. Although there are several competing algorithms for
achieving this goal, but Finite Difference Method (FDM) is used because of its simplicity [6]. A computational numerical simulation and modeling of Poisson equation for graded charge density in 1D was done by [7] and we will compare it with our results. In this paper, Poisson equation, which describe the potential at each grid point inside the device [8] was modeled in 2D for an abrupt charge density and linearly graded density systems with arbitrary points in space.

2. METHODOLOGY
A semiconductor solar cell is based on a simple p-n junction. The five equations that describe the behaviour of charge carriers in semiconductors under the influence of an electric field and/or light, both of which cause deviations from thermal equilibrium situations [9] can be expressed in equations 1 to 4.

\[
\frac{\partial V(x, y)}{\partial x^2} + \frac{\partial V(x, y)}{\partial y^2} = \frac{-\rho + n - \sum p - n}{\varepsilon} [p^n + n_T - N_D^+ + N_A^-]
\]

\[V(x, y)\] is the electrostatic potential, \(\varepsilon\) is the permittivity of free space, \(p\) is the concentration of holes, \(n\) is concentration of electrons, \(\rho\) is charge density, \(p_T\) and \(n_T\) are total concentration of holes and electrons respectively and \(n_D^+\) and \(n_A^-\) are donor and electron concentrations.

\[J_\text{e} = -\frac{\mu_e n E + e D_e \nabla n}{q} \]

\[J_\text{h} = -\frac{\mu_h p E + e D_h \nabla p}{q} \]

\(\mu_e\) and \(\mu_h\) are electron and hole mobility, \(D_e\) and \(D_h\) are electron and hole diffusion coefficients. \(E\) is electric field, \(J_e\) and \(J_h\) are electron and hole current density respectively.

\[
\frac{1}{q} \left( \frac{\partial^2 J_\text{e}}{\partial x^2} + \frac{\partial^2 J_\text{e}}{\partial y^2} \right) = G_n - R_n
\]

\[
-\frac{1}{q} \left( \frac{\partial^2 J_\text{h}}{\partial x^2} + \frac{\partial^2 J_\text{h}}{\partial y^2} \right) = G_p - R_p
\]

Where \(G_n\) and \(R_n\) are position dependent volume recombinations and photo generation rates respectively for electrons and \(G_p\) and \(R_p\) for holes, \(q\) is electronic charge.

But, in this work, Poisson equation was modeled in two dimensions. This is the foundation, in which continuity equations are solved and thereby been able to solve both transport and continuity equations which one can use the combination of these solutions to calculate the solar cell efficiency [9, 10].

2.1. Discretisation of 2D Poisson Equation

Since it is this equation that tells us about electric potential whose unit is joules per coulombs. And Joules is a measure of energy. Computational simulation will be utilized in order to model the behavior of complex geometry with practical values.
\[ \nabla^2 V(x, y) = -\frac{\rho(x)}{\varepsilon} \quad (6) \]

Defining a mesh grid of spatial points at which the voltage function will be sampled, if \( H_x = \) Vertical Distance, \( H_y = \) Horizontal distance and the point that lie on the mesh may be defined by \( x = iH_x, y = iH_y \)

\[ V(i, j) = V(x, y) \]

\[ \rho(i, j) = \rho(x, y) \]

\[ \frac{\partial^2 V(x, y)}{\partial x^2} + \frac{\partial^2 V(x, y)}{\partial y^2} = -\frac{\rho}{\varepsilon} \quad (7) \]

Then, applying three point approximation for the second derivative to both part of equation above

\[ \frac{\partial^2 V(x, y)}{\partial x^2} = \frac{V_{(x+h,y)} - 2V_{(x,y)} + V_{(x-h,y)}}{h_x^2} \quad (8) \]

\[ \frac{\partial^2 V(x, y)}{\partial y^2} = \frac{V_{(x,y+h)} - 2V_{(x,y)} + V_{(x,y-h)}}{h_y^2} \quad (9) \]

Combining the two equations give

\[ \frac{\partial^2 V(x, y)}{\partial x^2} + \frac{\partial^2 V(x, y)}{\partial y^2} = \frac{V_{(x+h,y)} - 2V_{(x,y)} + V_{(x-h,y)}}{h_x^2} + \frac{V_{(x,y+h)} - 2V_{(x,y)} + V_{(x,y-h)}}{h_y^2} \quad (10) \]

\[ V_{k+1} - (1+\lambda)V_k + V_{k-1} + \lambda V_{k+N_x} + \lambda V_{k-N_x} = V_k \quad (11) \]

Where \( k = (j-1)N_x, \lambda = \frac{h_x^2}{h_y^2} \)

The expression above means \( V(k) \) depends only on \( \rho(k) \) and voltage at the few nearest neighbors. Expressing the linear relationship between voltage samples into matrix \( A \) gives \( AV = B \) \[ 2, 10-13 \], \( B \) contains all the information about any charge densities and boundary conditions.

2.2 Boundary Conditions

In order to arrive at a unique solution, some boundary conditions were considered;

I. Newman Boundary condition was applied here. At the sides of the solar cell, \( V_{x=1} = V_x, V_{x=N} = 0 \) and \( \frac{\partial V}{\partial x} = 0 \)

II. At the top of the cell, the upper potential would be 2.0 while the lower potential should be zero. (Dirichlet boundary condition)
We assumed there are 16 points in space, i.e k=16, using eqn 11, the values of electric potential at each point in the cell is written in equation 12a – 12p

\[ V_1 = V_2 - (1 + 2\lambda)V_1 + \lambda V_3 = -\frac{\rho}{\varepsilon} \]  
\[ V_2 = V_3 - (1 + 2\lambda)V_2 + \lambda V_4 = -\frac{\rho}{\varepsilon} \]  
\[ V_3 = V_4 - 2(1 + \lambda)V_3 + \lambda V_7 = -\frac{\rho}{\varepsilon} \]  
\[ V_4 = -(1 + 2\lambda)V_4 + V_3 + \lambda V_6 = -\frac{\rho}{\varepsilon} \]  
\[ V_5 = V_6 - (1 + 2\lambda)V_5 + \lambda V_9 + \lambda V_1 = -\frac{\rho}{\varepsilon} \]  
\[ V_6 = V_7 - 2(1 + \lambda)V_6 + V_5 + \lambda V_{10} + \lambda V_2 = -\frac{\rho}{\varepsilon} \]  
\[ V_7 = V_8 - 2(1 - \lambda)V_7 + V_6 + \lambda V_{11} + \lambda V_3 = -\frac{\rho}{\varepsilon} \]  
\[ V_8 = -(1 + \lambda)V_8 + V_7 + \lambda V_{13} + \lambda V_4 = -\frac{\rho}{\varepsilon} \]  
\[ V_9 = V_{10} - (1 + \lambda)V_9 + \lambda V_{13} + \lambda V_5 = -\frac{\rho}{\varepsilon} \]  
\[ V_{10} = V_{10} - 2(1 + \lambda)V_{10} + V_8 + \lambda V_{14} + \lambda V_6 = -\frac{\rho}{\varepsilon} \]  
\[ V_{11} = V_{10} - 2(1 - \lambda)V_{11} + V_{12} + \lambda V_{13} + \lambda V_7 = -\frac{\rho}{\varepsilon} \]  
\[ V_{12} = -(1 + 2\lambda)V_{12} + V_{11} + \lambda V_{16} + \lambda V_8 = -\frac{\rho}{\varepsilon} \]  
\[ V_{13} = V_{14} - (1 + 2\lambda)V_{13} + \lambda V_9 + 2\lambda = -\frac{\rho}{\varepsilon} \]  
\[ V_{14} = V_{15} - 2(1 + \lambda)V_{14} + V_{13} + \lambda V_{10} + 2\lambda = -\frac{\rho}{\varepsilon} \]  
\[ V_{15} = V_{16} - 2(1 + \lambda)V_{15} + V_{14} + \lambda V_{11} + 2\lambda = -\frac{\rho}{\varepsilon} \]  
\[ V_{16} = -(1 + 2\lambda)V_{16} + V_{15} + \lambda V_{12} + 2\lambda = -\frac{\rho}{\varepsilon} \]

A MATLAB program was developed to solve this discretized Poisson equation with the above boundary conditions when Finite Difference Method was used. This program calculates the potentials in the problem domain.

3. RESULTS AND DISCUSSION
The results gotten from the simulation with MATLAB are plotted as in Fig. 1 and Fig. 2.
Figure 1 shows the abrupt p-n junction plot, and also the potential at each grid point across the depletion region of the solar cell. The maximum potential is at the edge of depletion region (the yellow part). This potential decreases smoothly reaching zero at midpoint of the region, and change polarity reaches the maximum at the other edge of depletion region. This is the barrier voltage in which the carrier must overcome the barrier in order to cross to the other side. In short, the doping type changes over a small distance compared to the extent of the depletion region, we assumed positive charge is in N region and negative charge in P region.
Fig. 1. The abrupt p-n junction plot

Figure 2 is a linearly graded p-n junction which shows the potential curve at each grid point across the depletion region of the solar cell with unequal concentration (a linearly graded). Linearly graded junction has a doping profile, which depends linearly on the distance from the interface.

\[ N_d - N_a = ax \]

\( N_d \) is density of donors, \( N_a \) is density of acceptors.

The depletion layer depends on in built potential this in turn depends on the depletion layer. The maximum potential is at the centre where the point charge was placed and decreases smoothly as it goes farther to the edges of the region. It was also noticed that the system was not affected when the number of grid points were increased, but rather the better it was and the higher the value of electric potential.
4.0 CONCLUSION
One of the governing equations of solar cells has been solved numerically. This work has modeled Poisson Equation in 2D for an abrupt and linearly graded charge densities system with arbitrary point in space. A general purpose semiconductor device simulator that is functional and modular in nature has also been developed. Some characteristics can be found, such as Electric potential, space charge density, carrier density and electric field, for the two doping densities. And also a tool that can supplement solar cell modeling, semiconductor physics and construction of basic solar cell device equation using MATLAB tool has been done successfully. However, the study can be extended to 3D to check whether the results will come faster and more accurate.

Fig. 2. Linearly Graded Charge Density plot
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