THE IMPLEMENTATION OF FINITE DIFFERENCE MINORITY CARRIER DIFFUSION EQUATION TO DETERMINE PM-147/SI BETAVOLTAIC PERFORMANCE

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Abstract. In this article, we employ a numerical calculation to determine the Pm₂O₁₇-Si p-n junction betavoltaic electrical performance using Finite Difference Minority Carrier Diffusion Equation (FD-MCDE) method. In order to verify the method, the comparison result is presented according to the basic planar design in the experimental study as well as the analytical calculation. At 0.8 Ci/cm² and 1 Ci/cm² activity content, we obtained 8.04% and 7.03% error in short-circuit current calculation, respectively. Furthermore, the variation in the number of n-type and p-type arrays was done to detect the shifting effect in the simulation result. The \( V_{oc} \), \( V_{mp} \), and \( FF \) for both activity contents have achieved the optimum values using 500 x 500 grids, despite of having more iterations to reach the desired convergency level.

1. Introduction

About several years ago, we were introduced to semiconductor device which became the driving force of microsystems technology development until this day. On the other hand, the development of microenergy source seems to face some difficulties. The issue includes several aspects of providing a high power density and long-lasting power source in a very small volume [1]. A betavoltaic battery is a kind of nuclear battery which requires no conversion of radiation-thermal-electricity like any other operating nuclear energy storage, such as RTG, or SRG. This device converts the decay energy directly into electricity by using semiconductor, similar to photovoltaic operation. Having a high power density in a small space, this battery could be one of the candidate of promising microenergy sources. Early discovery of electron induced voltage in semiconductor came out as an offspring of photovoltaic cell research and development. The description of electro-voltaic effect were first described in 1951 [2], where current magnification was observed in selenium photocells when they were bombarded by an electron beam. Subsequently, the first betavoltaic cell was introduced in 1954, wherein the beta source consists of Sr⁹₀-Y⁹₀ was coupled with p-n junction silicon device [3]. From those early experiments, it concludes that the beta particles emitted from decaying nuclides can be employed to generate electricity instead they have charges unlike photon. The radioisotope source has the energy density about \( 10^{2}-10^{4} \) times greater than fossil or chemical fuels, and it can be used for long-term application. Furthermore,
the source used in this nuclear battery is a low emitting isotope and leaves no harm to the environment, even it is safe to be implanted inside humans as the energy storage for cardiac pacemakers [4].

There have been several researches conducted in the theoretical study of betavoltaic battery: analytical study using silicon p-n junction with Ni-63 [4], using selective emitter micro battery [5], comparative study with Ni-63 and Pm-147 [6], using large-grain polysilicon [7], using 4H-SiC Schottky diode [8], and prediction using silicon p-n junction with Sr-90 [9]. All of those studies provides different approach, according to the type of semiconductor used as a radiation-electricity converting. For example, in p-n junction type of battery, the operational principle of semiconductor can be determined simply by analysing minority carrier diffusion [4], [6], [9]. The generation of electron-hole pairs is determined by the energy deposition of beta particles inside the materials. However, the theoretical approach of minority carrier diffusion equation is capable to analyse 1-D structure of betavoltaic such as basic planar in Figure 1(a), but for the 2-D structure such as the deep trenches model in Figure 1(b), it becomes more difficult to get the solution due to the variation of boundary condition.

In this article, we implemented a numerical approach using finite difference (FD) method to solve the minority carrier diffusion equation (MCDE) for 2-D calculation. The cell was divided into an array of tiny grids, with the respective boundary condition at the surfaces of n-type and p-type regions, and the edge of depletion region. As a preliminary study, we used the basic planar design using Pm-147/Si configuration from a previous experimental study [10]. Furthermore, we compare our results with the 1-D analytical approach using our previous analytical method [9].

![Figure 1](image_url)
2. Basic principle of betavoltaic battery

The beta particles can interact both with electron orbital and nuclei as long as they still have energy to penetrate the material and then stopped at certain range. Some of their kinetic energy are transferred to the electron orbital which causing the electron excited or ionized into a higher energy states, leaving hole at the atom. These electron-hole pairs would be swept away by the electric field and then generating current at the junction. Furthermore, the path of beta particles could be deflected from its incident angle, as a result of their interaction with the coulomb field of nuclide. The total energy degradation per depth can be expressed as follows [6]:

\[
\frac{dE}{ds}_{\text{total}} = \frac{dE}{ds}_{\text{ion}} + \frac{dE}{ds}_{\text{rad}}
\]  

(1)

The first part of the above expression is the degradation of kinetic energy caused by ionization process, which can be described by the analytical equation as follows [6]:

\[
\frac{dE}{ds}_{\text{ion}} = \frac{4\pi e^4}{m_0 v^2} Z N \left( \ln \frac{2m_0 v}{I} + 1.2329 \right)
\]  

(2)

where \(Z\) is the total atomic number of the absorber, \(N\) is the atomic density of the absorber, \(m_0\) is the rest mass of particle, \(v\) is the average velocity of the particle inside the absorber, and \(I\) is the mean ionization and excitation number of the absorber. Subsequently, the second part is defined as the energy loss due to the nuclei interaction which can be described by the analytical equation as follows:

\[
\frac{dE}{ds}_{\text{rad}} = \frac{NEZ(Z+1)^4}{137m_0^2 c^4} \left( 4 \ln \frac{2E}{m_0 c^2} - 1.333 \right)
\]  

(3)

Since the average kinetic energy of typical beta particles used for betavoltaic device is in the Kilo Electron Volt (keV) range, a single beta particle is responsible for generating multiple EHPs. The Klein Formula describes that the average kinetic energy required to generate an EHP is equal to sum of the semiconductor band-gap (\(E_g\)) and the vibration energy (\(E_{ph}\)). During the conversion process, there is some energy lost in the process of acoustic and optical phonons emission or absorption, depends on the structure of semiconductor crystallinity [11].

\[E_{\text{ph}}(x) = E_{\text{ph}} \exp(-\alpha x)\]

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Figure 2. Beta spectra of Pm-147 radioisotope.

Figure 3. Energy deposition of beta particles emitted from Pm-147 along the depth of silicon. The red-squared lines is the MCNP simulation result and the blue line is the exponential fitting.
In contrast to the alpha particle, the beta particle from a given radioactive nuclide is not emitted in a discrete energy group, instead of a continuous energy distribution extending from zero to maximum value [12]. The spectrum of beta particles emitted from Pm-147 is shown in Figure 2, which is used to define the isotropic emission from the source. Monte Carlo N-Particle code was used to simulate the energy deposition by employing tally *F8: E* (pulse height tally of electron). Figure 3 shows the energy deposition value from the simulation (red-squared line) and the fitting result using exponential decay model, we obtained $E_{\beta 0} = 0.1816$ and $\alpha = 387.5$. These fitting coefficients were used to describe the degradation of beta energy per depth later.

3. FD-MCDE for betavoltaic operation

According to photovoltaic theory, the minority carrier diffusion equation can be used to determine the short-circuit current generated along the p-n junction regions by analysing the carrier generation and recombinaction [13]. The generation rate of betavoltaic cell can be represented by this following formula:

$$G(s) = \Phi_0 (1 - R) \frac{(dE/ds)_{iso}}{2.86E_g + E_{\beta}}$$

(4)

where $\Phi_0$ is the incident flux on the surface of absorber, and $R$ is the reflection coefficient. However, due to the isotropic emission of the source, it is convenient for the basic planar design to assume that only 50% of the source activity is responsible for generating EHPs.

The time-independent MCDE for both electron and hole can be described by these following formulas, respectively:

$$D_n \left( \frac{\partial^2 \Delta n(x,y)}{\partial x^2} + \frac{\partial^2 \Delta n(x,y)}{\partial y^2} \right) - \frac{\Delta n(x,y)}{\tau_n} + G(x,y) = 0$$

(5)

$$D_p \left( \frac{\partial^2 \Delta p(x,y)}{\partial x^2} + \frac{\partial^2 \Delta p(x,y)}{\partial y^2} \right) - \frac{\Delta p(x,y)}{\tau_p} + G(x,y) = 0$$

(6)

where $\Delta n(x,y)$ and $\Delta p(x,y)$ is the electron and hole concentration on the specified area, $D_n$ and $D_p$ is the diffusion coefficient of electron and hole, $\tau_n$ and $\tau_p$ is the electron and hole lifetime before they recombine. Applying the finite difference method, the numerical solution to the above equations become:

$$\Delta n_{i,j}^{k+1} = \frac{\Delta n_{i+1,j}^{k} + \Delta n_{i-1,j}^{k} + \left( \frac{\Delta x}{\tau_n} \right)^2 (\Delta n_{i,j+1}^{k} + \Delta n_{i,j-1}^{k}) + \left( \frac{\Delta y}{\tau_n} \right)^2 \Delta n_{i,j}^{k}}{2 \left( \frac{\Delta x}{\tau_n} \right)^2 + \left( \frac{\Delta y}{\tau_n} \right)^2}$$

(7)

$$\Delta p_{i,j}^{k+1} = \frac{\Delta p_{i+1,j}^{k} + \Delta p_{i-1,j}^{k} + \left( \frac{\Delta x}{\tau_p} \right)^2 (\Delta p_{i,j+1}^{k} + \Delta p_{i,j-1}^{k}) + \left( \frac{\Delta y}{\tau_p} \right)^2 \Delta p_{i,j}^{k}}{2 \left( \frac{\Delta x}{\tau_p} \right)^2 + \left( \frac{\Delta y}{\tau_p} \right)^2}$$

(8)

The index of $i$ represents the column position of the grid and $j$ as the row. The index of $k$ represents the number of iteration in the calculation. If the calculation value on the respective grid still above the threshold error, the iteration occurs. Figure 4 shows the illustration of the p-n junction area which had been divided into tiny grids with the desired geometry.
Figure 4. Illustration of the numerical grid used for the cell simulation.

In order to find the most optimum value according to the real measurement, the total array of the n-type and p-type regions were varied by 100 x 100, 200 x 200, 300 x 300, 400 x 400, and 500 x 500 separately. The number of iteration is also taken into account, as we want to know the effectiveness of the array variations. The depletion region current is neglected for this situation, as it only occupied the smallest space on the p-n junction area (according to the doping level concentration parameters).

Table 1. Basic semiconductor parameters of the device.

| Parameter                        | Value |
|----------------------------------|-------|
| p-Type width (cm)                | Wp    | 0.01784 |
| n-Type width (cm)                | Wn    | 7.998E-05 |
| Depletion width (cm)             | Wd    | 7.619E-05 |
| Total thickness (cm)             | Wp+Wn+Wd | 0.018 |
| n+ doping concentration (/cm³)   | N_d   | 1E+20 |
| p+ doping concentration (/cm³)   | N_a   | 2E+15 |
| Dark saturation current density  | J_o1  | 1.642E-15 |
| Surface area (cm²)               | A     | 2.85   |
| Reflection coefficient           | R     | 0.17   |

In this study, we used the reference design (Device 1) of betavoltaic cell from [10] to verify that our calculation are satisfying with both their real measurement and their simulation study. According to the reference, the design consists of a silicon based planar p-n junction coupled with Pm₂O₃ radioisotope source, each had five different activity content but in this study we only used two different activity content for this simulation. The semiconductor parameters are listed in Table 1. The dark saturation current density was calculated manually using doping level concentration data and theoretical derivation of photovoltaic analysis in [14].

4. Results and Discussions

The objective of this work is to develop the FD-MCDE method and verify the simulation results with the real measurement results. In this work, we implemneted 0.8 Ci/cm² and 1.0 Ci/cm² activity content for the Pm₂O₃ source. For each activity content, we also calculated the electrical performace using analytical MCDE with our previous model in [9]. The results from our simulation work will be discussed further in this section.
4.1 Validation to the analytical simulation

To begin with, we used 100 x 100 array for both n-type and p-type regions to simulate the cell operation. The short-circuit current ($I_{SC}$) is equal to the sum of current at the p-type and n-type regions. For every regions, the current can be determined by looking at the gradient at the edge of each junctions. The I-V curve and P-V curve can be drawn by implementing the equation as follows, respectively:

\[ I(V) = I_{SC} - I_{01} \exp \left( \frac{qV}{kT} - 1 \right) \]  
\[ P(V) = V \left[ I_{SC} - I_{01} \exp \left( \frac{qV}{kT} - 1 \right) \right] \]

where $I_{01}$ is the dark saturation current, $q$ is the charge of electron, $V$ is the voltage, $k$ is the Boltzmann constant, and $T$ is the temperature of operation (room). Figure 5 shows the result of I-P-V curves using the described equations.

![Figure 5](image.png)

**Figure 5.** The I-P-V curves of betavoltaic simulation using two activity content with $^{147}$Pm$_2$O$_3$ source. The simulation results at (a) was done using analytical MCDE method, and (b) using FD-MCDE method.

As shown in Figure 5(a), the I-P-V curves from analytical method have a slightly higher values than in Figure 5(b) from FD method for both activity content. However, in the FD-MCDE methods the current generated in depletion region was not calculated, thus reducing the total current although it is not giving a significant impact.
From the real measurement in [10], they reported that $I_{sc}$ for 0.8 Ci/cm$^2$ activity content is about 27 $\mu$A, and for 1.0 Ci/cm$^2$ activity content is about 29 $\mu$A. From Figure 6(a), it can be seen that $I_{sc}$ from the FD-MCDE method gives slightly lower value than the analytical MCDE calculation where at the first activity content $\Delta I_{sc} = 1.257 \mu$A and the second one $\Delta I_{sc} = 1.572 \mu$A. In comparison to the real measurement, at the 0.8 Ci/cm$^2$ the analytical calculation has a closer result than the FD-MCDE calculation, but the condition is reversed at the 1.0 Ci/cm$^2$. The deviation from simulation is occurred due to some factors, including the surface recombination velocity was set to zero (ideal ohmic contact) for both surfaces, no parasitic resistance effects, and other unideality in experimental conditions that have been neglected from simulation.

![Comparison chart of $I_{sc}$ from the analytical and FD-MCDE simulation with the real measurement data from [10]: (a) the value of $I_{sc}$, and (b) percentage of error in $I_{sc}$.](image)

**Figure 6.** Comparison chart of $I_{sc}$ from the analytical and FD-MCDE simulation with the real measurement data from [10]: (a) the value of $I_{sc}$, and (b) percentage of error in $I_{sc}$.

### 4.2. Variation in number of arrays

In this section, the electrical performance of betavoltaic would be discussed by using different number of n-type and p-type arrays. The initial condition of $\Delta n(i,j)$ and $\Delta p(i,j)$ of each individual cell was set to zero. One of the key feature of this FD-MCDE method is the agility and flexibility of setting the boundary condition related to the structure. In this simulation, the boundary condition was set using junction edge principle described in [14]. The iteration would continue until $|\Delta p^k - \Delta p^{k+1}| < 1E-5$ for n-type cell and $|\Delta n^k - \Delta n^{k+1}| < 1E-5$ for p-type cell.

| Number of arrays | 100 x 100 | 200 x 200 | 300 x 300 | 400 x 400 | 500 x 500 |
|------------------|-----------|-----------|-----------|-----------|-----------|
| $k$              | 7565      | 28196     | 60711     | 125326    | 194388    |
| $I_{sc}$ ($\mu$A)| 24.831    | 25.449    | 25.654    | 25.760    | 25.823    |
| $V_{oc}$ (Volt)  | 0.4396    | 0.4403    | 0.4405    | 0.4406    | 0.4406    |
| $I_{mp}$ ($\mu$A)| 23.199    | 23.779    | 23.978    | 24.078    | 24.135    |
| $V_{mp}$ (Volt)  | 0.3691    | 0.3696    | 0.3698    | 0.3699    | 0.3700    |
| $P_{mp}$ ($\mu$W)| 8.563     | 8.791     | 8.867     | 8.906     | 8.929     |
| FF               | 0.784     | 0.785     | 0.785     | 0.785     | 0.785     |

The electrical performance parameters at 0.8 Ci/cm$^2$ with the variation in the number of arrays are listed in Table 2. As the total number of arrays increased, so does the overall electrical performance,
slowly approaching the analytical calculation result. The $V_{oc}$, $V_{mp}$, and $FF$ values have reach the saturation point, while on the other hand there are still a traceable alteration in $I_{sc}$, $I_{mp}$, and $P_{mp}$ values although it is insignificant. Furthermore, the escalation in the total number of arrays also increases the iteration required for the calculation, thus the computing time would also be increased. In this case, the escalation have brought $I_{sc}$ value closer to the real measurement.

Table 3. Simulated betavoltaic electrical performance at 1.0 Ci/cm$^2$ activity content with different number of n-type and p-type arrays.

| Number of arrays | 100 x 100 | 200 x 200 | 300 x 300 | 400 x 400 | 500 x 500 |
|------------------|-----------|-----------|-----------|-----------|-----------|
| $k$              | 7649      | 28528     | 61459     | 126124    | 195878    |
| $I_{sc}$ ($\mu$A) | 31.039    | 31.801    | 32.066    | 32.199    | 32.279    |
| $V_{oc}$ (Volt)  | 0.4454    | 0.4460    | 0.4462    | 0.4463    | 0.4464    |
| $I_{mp}$ ($\mu$A) | 29.0295   | 29.745    | 29.993    | 30.119    | 30.199    |
| $V_{mp}$ (Volt) | 0.3745    | 0.3751    | 0.3753    | 0.3754    | 0.3754    |
| $P_{mp}$ ($\mu$W) | 10.8715   | 11.157    | 11.256    | 11.306    | 11.336    |
| $FF$             | 0.786     | 0.787     | 0.787     | 0.787     | 0.787     |

At 1.0 Ci/cm$^2$ activity content, the electrical performance of betavoltaic is also increased as the total number of arrays increases as shown in Table 3. Generally, the total iteration required to reach the same optimum level is higher than 0.8 Ci/cm$^2$ activity content, despite only having small amount of difference. The $V_{oc}$, $V_{mp}$, and $FF$ values have also saturated. However, the escalation of the total number of arrays in this case did not improve the aucracy of simulation result to the real measurement. In order to fix this situation, we could adjust the boundary condition at the front and the back surface with the real situation in the measurement, analyze the leakage current generated by thermal recombination, or measure the parasitic resistance of the betavoltaic cell. Furthermore, the study of apparent activity and the self-absorbance from the source itself should be conducted since it is a critical aspect to analyse the generation of electron-hole pairs.

5. Conclusion

Using the FD-MCDE method, the betavoltaic electrical performance has been succesfully simulated. In comparison to the analytical calculation, the results show that for 0.8 Ci/cm$^2$ activity content $\Delta I_{sc} = 1.257 \mu$A, and for 1.0 Ci/cm$^2$ activity content $\Delta I_{sc} = 1.572 \mu$A. Furthermore, we obtained that calculation error for 0.8 Ci/cm$^2$ and 1.0 Ci/cm$^2$ activity content is about 8.04% and 7.03%, respectively. The improvement in the total number of arrays was done, and generally the betavoltaic electrical performance from two activity contents using FD-MCDE method have reach the optimum value for $V_{oc}$, $V_{mp}$, and $FF$. On the other hand, the iteration required for the calculation is also increased, thus increasing the time required to solve the FD-MCDE calculation. Some factors excluded from the simulation such as surface boundary conditions, or other sources of leakage current should be taken into account to match the real condition.

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