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Evaluation of GEANT4 and COMSOL Multiphysics Coupling Capabilities by Simulation of an Optimized Betavoltaic Battery

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ABSTRACT
A beta-voltaic battery design can be used to evaluate the functionality of the GEANT4 code and COMSOL Multiphysics software. The spatial distribution of the deposited energy for the beta particles in the semiconductor transducer has been simulated by using the GEANT4 and then, the electron-hole pair generation rate has been obtained. Subsequently, output performances of the battery such as the current-voltage (I–V) characteristics and the maximum electrical power have been determined by using the COMSOL Multiphysics in which the electron-hole pair generation rate from the GEANT4 simulation was utilized as input. Validation is done by considering an optimized planar betavoltaic battery. The results of the current study have been compared with other articles. The results are in good agreement and the relative errors are less than 8%. Our simulation model can be extended to the betavoltaic batteries with other semiconductors and radioactive isotopes and can provide a powerful tool for predicting the output performance and optimizing the betavoltaic batteries.

***Keywords*:** Simulation; Model; Geant4; COMSOL Multiphysics; Betavoltaic Battery

1. Introductions

Several methods and tools have been used in the design of betavoltaic batteries. In related published papers, simulation software such as Synopsys, Silvaco, and Comsol has been used in semiconductor design as a betavoltaic battery converter [1-7]. The finite element method (FEM) is one of the efficient computational methods in engineering and applied science. Modern computational methods, such as FEM, and advanced modeling software tools, such as COMSOL, are valuable resources for solving complex engineering problems as well as optimizing our designs to have more economical, reliable, and durable products as results [8].

An important part designing betavoltaic battery devices is to understand the proper functioning of the involved processes. It is essential to take a detailed observation of the physical processes that

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take place inside the battery, especially carrier transport and collection characteristics. This can help in explaining the effects of structure parameters on battery performance and lead to optimization. The Semiconductor Module extends the functionality of the physics interfaces in the base package for COMSOL Multiphysics. It is a collection of interfaces and predefined models for COMSOL Multiphysics which can be used to model semiconductor devices [9].

One of the advantages of using COMSOL software in semiconductor design and extraction of electrical parameters is that it makes it possible to enhance by changing the design parameters. It also has the ability to combine with other computational codes. Combining this software with the Geant4 code to simulate nuclear radiation transport provides researchers with many capabilities for designing and optimizing betavoltaic batteries.

Tang et al. performed a theoretical calculation model for planar betavoltaic batteries using the semiconductor material, Si, and radioisotope, ^{63}Ni. Using the Monte Carlo N-Particle (MCNP) code, we were able to simulate the transport of beta particles in semiconductor materials and obtain the formulas for nuclear radiation current, open circuit voltage, and other calculations [10]. Maleki and Etaati simulated these micro-betavoltaic battery characteristics by the MCNPX-SILVACO hybrid code [11].

In this paper, we have developed a realistic model to optimize the betavoltaic battery design. The realistic betavoltaic nuclear battery based on ^{63}Ni/Si has been simulated by coupling the Geant4 code and COMSOL Multiphysics software. Beta particles transport and electron-hole pair (EHP) generation rate were calculated by using Geant4 code and as an input file imported to COMSOL Multiphysics software and then output performances of the betavoltaic batteries were determined. The user-defined spatially dependent variable for electron-hole pair generation rate has been determined in COMSOL Semiconductor Module. Comparing the simulation results with other works [10, 11] has been undertaken to ensure accuracy.

2. Theoretical Foundations

Coupling Geant4 code with COMSOL Multiphysics software empowers to simulation of both the semiconductor and beta source parts. It also promotes electron-hole pair generation in Si semiconductors. A worthy estimation of the electron absorption behavior in the silicon, as a transducer of betavoltaic battery, can be determined by Geant4 Monte Carlo simulations. Geant4 is a free software package composed of tools that can be used to accurately simulate the transport of nuclear particles through matter [12]. Klein gives the total energy dissipated per electron-hole pair produced $\varepsilon = 2.8E_g + 0.5$, where E_g is the bandgap of the semiconductor [13]. The generation rate of electron-hole pairs G(y) is given by

$$G(y) = \frac{E_{dep}}{\varepsilon} \tag{1}$$

Where E_{dep} is the energy absorbed by electronic interactions at a distance y in the Semiconductor [14]. The ionization energy deposition is obtained by Geant4 and converted into the generation rate of EHPs and mapped to COMSOL Multiphysics software, to simulate the output characteristics of silicon PN betavoltaic batteries. The semiconductor device was designed using the Semiconductor Module of COMSOL Multiphysics software. The Semiconductor Module includes a predefined Semiconductor interface, which is based on the conventional drift-diffusion formulation. Also, an optional density-gradient implementation is available to provide a computationally efficient method to add the effect of quantum confinement to the drift-diffusion equation system. In addition, a predefined

Schrödinger Equation interface and a predefined Schrödinger-Poisson Equation Multiphysics interface allow more detailed modeling of quantum-confined systems such as quantum wells, wires, and dots. The Semiconductor Module enables the stationary and dynamic performance of devices to be modeled in one, two, and three dimensions, together with circuit-based modeling of active and passive devices [15].

To model it, the geometry is first defined in the software, then appropriate materials are selected and the semiconductor interface is added. The dopant distribution can be computed separately using a diffusion equation calculation, imported from third-party software, or specified empirically using the built-in doping features. The physics interface is used to establish initial conditions and boundary conditions. Next, the mesh is defined and a solver is selected. Finally, the results are visualized using a wide range of plotting and evaluation tools. All of these steps are accessed from the intuitive COMSOL Desktop graphical user interface.The stationary study is selected in COMSOL Multiphysics software.

3. Structure Design

The betavoltaic battery operates at room temperature (300 K). The optimized design parameters of a planar betavoltaic are shown in Table 1.

Table 1. The optimized design parameters of a planar betavoltaic battery [10].

Parameter	Value
The mass thickness of radioisotope	1 mg/cm^2
The doping concentration of P-type	1×10^{19} cm^{-3}
The doping concentration of N-type	3.16×10^{16} cm^{-3}
Junction depth	0.3 µm
Junction area	1 cm^2
The total thickness of the battery	160 µm

Fig.1 shows the simulated planar betavoltaic battery in the Geant4 code. There is a representation of the backscattered particle trajectory and the deposited energy. The red lines stand for the trajectory of electrons and the yellow spots stand for the energy loss points.

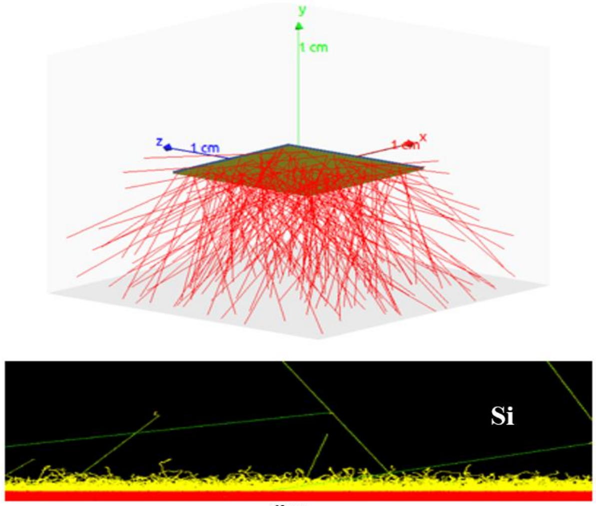

Fig. 1. Geant4 simulation setup for Si-^{63}Ni betavoltaic battery.

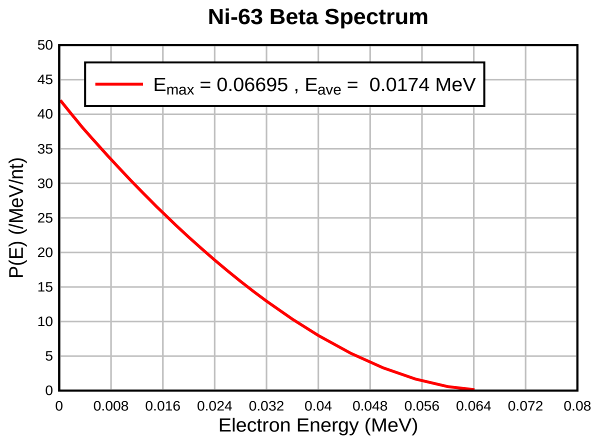

Fig. 2. Beta particles energy spectrum for ^{63}Ni.

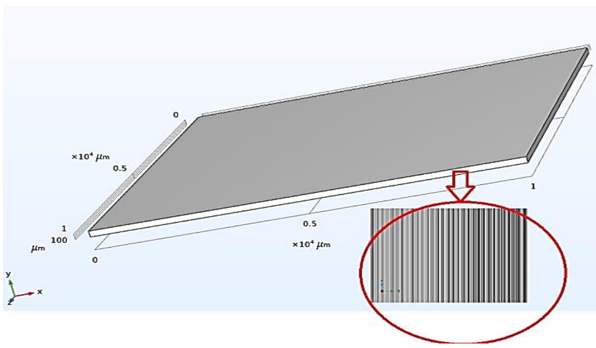

Fig. 3. 3-D schematic of the PN diode structure.

An accurate continuous beta energy spectrum was used for simulations of the beta emission source [16, 17]. The energy spectrum of beta particles for ^{63}Ni is shown in Fig. 2.

A 3-D schematic of the PN diode structure for betavoltaic cell and their mesh simulations in COMSOL Multiphysics is shown in Fig. 3.

The semiconductor properties of Si used in COMSOL Multiphysics software are listed in Table 2.

Table 2. Semiconductor properties of Si used in COMSOL Multiphysics simulations [18,19].

Parameter	Symbol	Value
Band gap	Eg	1.12eV
Electron affinity	χ	4.05 eV
Relative permittivity	ε_r	11.8
Effective density of states, valence band	N_c	2.86×10^{19} cm^{-3}
Effective density of states, the conduction band	N_v	3.10×10^{19} cm^{-3}
Minority electron mobility	μ_e	1450 cm^{2}V^{-1}s^{-1}
Minority hole mobility	μ_p	500 cm^{2}V^{-1}s^{-1}
Minority electron lifetime	τ_e	10μs
Minority whole lifetime	τ_p	10μs

4. Results and Discussion

The calculated electron-hole pair generation rate within silicon under the illumination of 100 mCi ^{63}Ni is shown in Fig. 4.

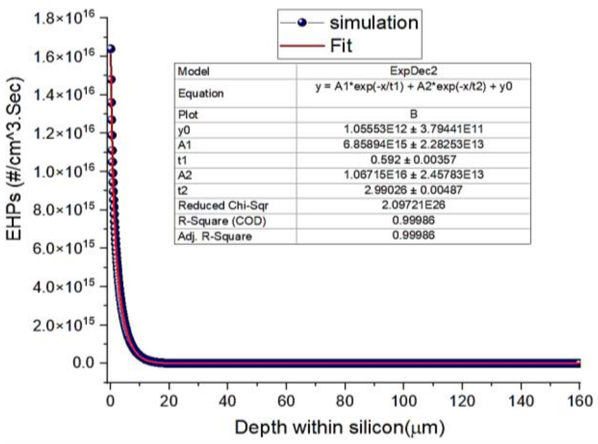

Fig. 4. EHPs generation rate within silicon under the illumination of ^{63}Ni.

In the COMSOL Multiphysics software, by sweeping the voltage across the PN diode and recording the terminal current, we can obtain the current-voltage (I–V) and power–voltage (P–V) characteristics of the betavoltaic battery. Fig.6 shows the I-V and P-V curves of the betavoltaic nuclear battery.

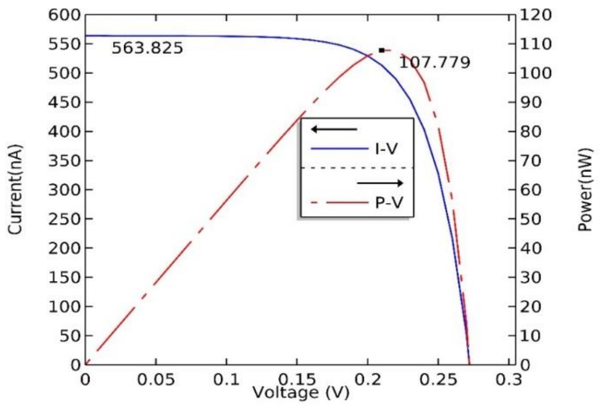

Fig. 5. I-V and P-V curves of the betavoltaic nuclear battery.

The electrical parameters of the betavoltaic battery, namely the short-circuit current (Isc), open-circuit voltage (Voc), fill factor (FF), and maximum electrical power (P_{max}), are calculated as 563.8 nA, 273mV, and107.78 nW, respectively. The conversion efficiency was 5.33%. Output simulation results have been compared with the data of Tang et al. and Maleki and Etaati are shown in Table 3.

Table 3. Comparison of the results with others.

Outputs	Tang et al.	Maleki and Etaati	This study	Relative error(%)
I_{sc}(nA)	573.3	596.8	563.8	1.66
V_{oc}(mV)	253	268	273	7.91
P_{max}(nW)	99.85	110.47	107.78	7.94
Fill factor(%)	68.84	69.07	70.02	1.71
Efficiency (%)	4.94	5.46	5.33	7.89

5. Conclusion

In this paper, a detailed model for a beta-voltaic battery based on Si is presented using the Geant4 code and the COMSOL Multiphysics software. We obtained the electrical parameters of the betavoltaic battery, including short-circuit current, open-circuit voltage, output power, and conversion efficiency, 563.8 nA, 0.273 V, 107.78 nW, and 5.33% respectively. The results are in good agreement with the others, and the differences are less than 8%. Our simulation model can be extended to the betavoltaic batteries with other semiconductors, radioactive isotopes, geometry, and structures, providing a powerful tool for predicting the output performance and optimizing the betavoltaic batteries.

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