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Evaluation of GEANT4 and COMSOL Multiphysics coupling capabilities by simulation of an optimized betavoltaic battery

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Abstract

In this research, we considered the isotropy of the incident beta particles, the self-absorption effect of the source, and the recombination effect on the performance of the betavoltaic nuclear battery by designing volumetric and coupling Geant4 and COMSOL Multiphysics. We developed a realistic model for optimizing betavoltaic battery design. For a case study of designing a planar betavoltaic battery That is, the mass thickness of radioisotope ^{63}Ni is 1 mg/cm^2, the doping concentration of the P-type region is 1×10^{19} cm^{-3} and that of N-type region is 3.16×10^{16} cm^{-3}, the junction area is 1 cm^2, the junction depth is 0.3 µm and the total thickness of the battery is 160 µm. We obtain maximum short-circuit current, open-circuit voltage, output power, and conversion efficiency, 563.8 nA, 0.301 V, 122.65 nW,and 6.06%, respectively. The results of the current study compared with two previous articles and the accuracy of the model is verified. Our simulation model can be extended to the betavoltaic batteries with other semiconductors and radioactive isotopes.

Keywords: Realistic Model, Geant4, COMSOL Multiphysics, Betavoltaic Battery

Introduction

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 finding solutions to complex engineering problems and optimizing our designs to have more economical, reliable, and durable products as end results[1].

An important part of designing betavoltaic battery devices is having a deep understanding of how the processes involved will work. It is necessary to take a detailed observation during the physical processes that take place inside the battery, especially carrier transport and collection characteristics. This can contribute to illuminating the effects of structure parameters on the battery performance, further guiding the optimization and fabrication. The Semiconductor Module extends the functionality of the physics interfaces of the base package for COMSOL Multiphysics. Its a collection of interfaces and predefined models for COMSOL Multiphysics, which can be used to model semiconductor devices[2].

In this paper, we developed a realistic model for optimizing betavoltaic battery design. we have simulated a realistic betavoltaic nuclear battery based on ^{63}Ni/Si by coupling Geant4 and COMSOL Multiphysics and compared the simulation results with Ref [3], Ref [4] to verify accuracy.

User-defined spatially dependent variable for electron-hole pair generation rate was determined in COMSOL Semiconductor Module. Beta particles transport and electron-hole pair generation rate were simulated by using Geant4 and were imported to COMSOL software and then the output performances of batteries are determined by using COMSOL Multiphysics.

Theoretical Foundations

Coupling COMSOL multiphysics with Geant4 empowers us to simulate the semiconductor and beta source and to estimate the distribution of electron-hole pair (EHP) generation in Si semiconductors. A good estimation of electron absorption behavior of silicon, as a transducer of betavoltaic battery, can be determined by Geant4 Monte Carlo simulations. The ionization energy deposition obtained by Geant4 is converted into the generation rate of EHPs and mapped to COMSOL Multiphysics software, to simulate the output characteristics of silicon PN betavoltaic microbatteries. The stationary study has been selected in COMSOL Multiphysics.

Structure design

The optimized design parameters of a planar betavoltaic battery have been given in Ref [3] shown in Table1. The battery operates at room temperature (300 K).

Table1.The optimized design parameters of planar betavoltaic[3].

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

Fig.1 shows the simulated planar betavoltaic battery in Geant4. The backscattered particle trajectories and deposited energy are also represented. the red lines stand for the trajectory of electrons and the yellow spots stand for the energy loss points.

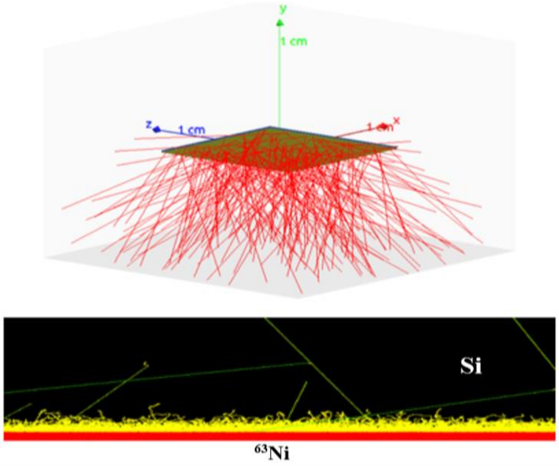


Figure 1. Geant4 simulation setup for Si-^{63}Ni betavoltaic nuclear battery.

An accurate continuous beta energy spectrum will be used for simulations in this paper [5,6]. The energy spectrum of beta particles of ^{63}Ni shown in Fig. (2)

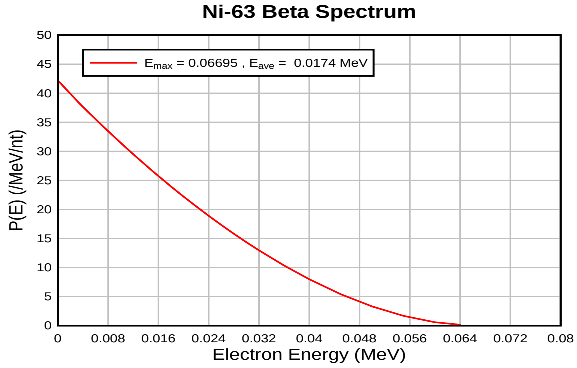


Figure 2. Continuous beta energy distributions for ^{63}Ni.

3-D schematic of the PN diode structure for betavoltaic (BV) cell and mesh simulation in COMSOL Multiphysics is shown in Fig. (3).

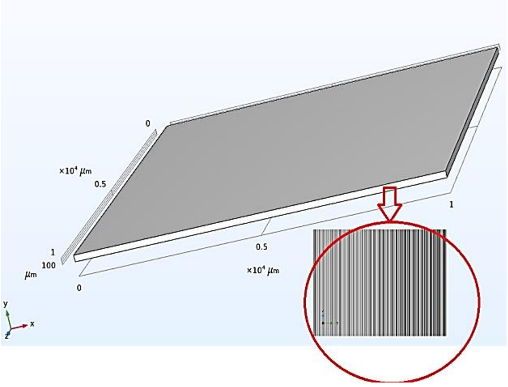
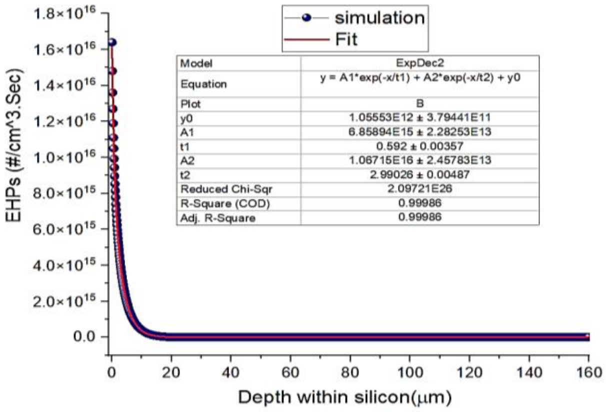


Figure 3. 3-D schematic of the PN diode structure.

Results and discussion

Calculated electron-hole pair(EHP) generation rate within silicon under the illumination of 100 mCi ^{63}Ni shown in Fig.(4)



Model	ExpDec2
Equation	y = A1*exp(-x/t1) + A2*exp(-x/t2) + y0
Plot	B
y0	1.05553E12 ± 3.79441E11
A1	6.85894E15 ± 2.28253E13
t1	0.592 ± 0.00357
A2	1.06715E16 ± 2.45783E13
t2	2.99026 ± 0.00487
Reduced Chi-Sqr	2.09721E26
R-Square (COD)	0.99986
Adj. R-Square	0.99986

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

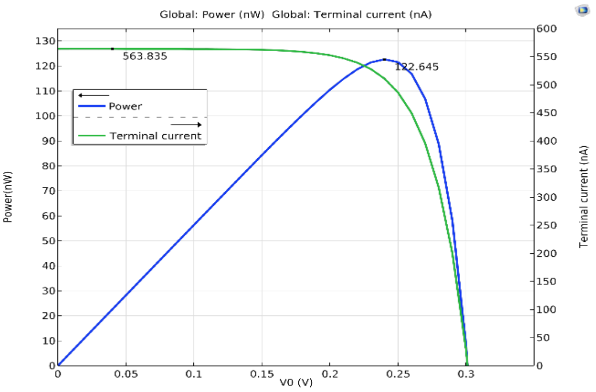


Figure 5. I-V and P-V curves of the betavoltaic nuclear battery.

Outputs simulation results are compared with the data of Ref [3] and [4] and are shown in Table 2.

Table 2. Compared simulation results with Ref [3] and Ref[4].

Outputs	Ref [3]	Ref [4]	This study

I_{sc}(nA)	573.3	596.8	563.8
V_{oc}(mV)	253	268	301
P_{max}(nW)	99.85	110.47	122.64
Fill factor(FF)	68.84	69.07	72.27
Efficiency (%)	4.94	5.46	6.06

Conclusions

This paper presents a detailed model based on Geant4 and COMSOL Multiphysics for a Si-based betavoltaic battery The accuracy of the model is verified by comparing it with Ref [3] and Ref [4]. we obtained maximum short-circuit current, open-circuit voltage, output power, and conversion efficiency, 563.8 nA, 0.301 V, 122.64 nW and 6.06% respectively. The results of this study have been compared with two previous Articles and The accuracy of the model is verified. Our simulation model can be extended to the betavoltaic batteries with other semiconductors and radioactive isotopes.

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