I-V- Characteristics analysis of betavoltaic microbatteries using TCAD model

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Abstract. The complete analysis of I-V characteristics and set of basic parameters for betavoltaic silicon batteries under Nickel-63 irradiation in the temperature range from 213 to 330 K is carried out using a universal physical TCAD model. The standard TCAD optical generation model was adopted for simulation of electron-hole generation for beta particles irradiation. The pn-junction diode energy converters with real Gaussian doping profiles are considered. The simulated current-voltage characteristics of the ⁶³Ni-Si betavoltaic elements are in good agreement with the measured characteristics.

1. Introduction

It is well known that conventional electrochemical batteries, widely used in electronic devices, have limited lifetime and tendency to degrade under hard environmental conditions [1]. There is a lot of applications in biomedical, aerospace, military, industrial, agricultural fields where battery replacement is impossible. In these cases, a low power (1µW- 10mW) and long lifetime (20-50 years) betavoltaic microbatteries are suitable as an alternative to electrochemical batteries. A betavoltaic battery is an electronic device which consists of two main parts: the radioisotope source and the converter transforming radioactive energy into electric current and/or voltage.

For a beta emitting isotopes, the beta energy and decay half-life time are the most important criteria. From this standpoint, the most perspective radioisotopes are Tritium, Nikel-63 and Promethium-147 (Table 1) [1].

As a converter which transforms radiation into electricity, the diode p-n junction structure is the simplest and the most popular for practical applications.

The basic mechanisms of conversion of radiation into electricity are shown in Figure 1. Beta particles collide with atoms and create electron-hole pairs (EHPs). One particle creates over 1000 EHPs and deposits some energy into the lattice. The electrical field in the depletion region accelerates the holes to the P-side contact and electrons to the N-side contact. As a result, the current flow appears through the connected load.

In choosing the semiconductor material for the pn-junction, the material density, band gap energy, and resistivity are important (Table 2) [2]. High bandgap materials exhibit high open-circuit voltage $V_{oc}$ and low reverse (dark) current $I_{dark}$. However, the higher resistivity materials have high defect density,
which reduces the conversion efficiency $\eta$.

The betavoltaic diodes typically generate currents on the order of nano- to micro-ampere. So, many betavoltaic cells with similar operating performance are stacked in parallel or in series to provide higher current or voltage, respectively [3]. Another perspective way is using 3D micro channel structures with deep trench radioisotope layers (Figure 2) [4-6].

Thus, the design of a betavoltaic microbattery with optimal output parameters is a topical issue. Available experience shows that only experimental methods are insufficient, modeling and simulation methods must be used as well. For this purpose, the TCAD models of the generation process of electron-hole pairs (EHPs) in betavoltaic [7-9] and carrier transport and collection processes within the PN-junction diode structure were used [10-12].

Unfortunately, only in few works, two types of models were coupled in a general system for complete betavoltaic modeling [8, 9]. Moreover, in all the publications, the PN-junction diode structures with simplified one-dimensional abrupt doping profiles were simulated, which introduced inaccuracy in the device performance modeling.

In this work, the complete analysis of I-V characteristics and set of basic parameters: short-circuit current density $J_{sc}$, open-circuit voltage $V_{oc}$, reverse (dark) current $I_{dark}$, output power density $P_{max}$, energy conversion efficiency $\eta$, for betavoltaic silicon batteries under Nickel-63 irradiation at normal temperature of 300 K and in the temperature range from 213 to 330 K is carried out using the universal physical 2D/3D TCAD model.

Table 1. The decay half-life time and beta particles energies of the most perspective radioisotopes

| Isotopes       | $T_{1/2}$ (yr) | $E_{avg}$ (keV) | $E_{max}$ (keV) | W/g | Cost/Ci |
|----------------|---------------|-----------------|-----------------|-----|---------|
| Tritium        | 12.36         | 6.0             | 18.6            | 0.33| $3.5$   |
| Nickel-63      | 100.00        | 18.0            | 65.9            | 0.006| $4.0$  |
| Promethium-147 | 2.62          | 60              | 230             | 0.37| $1.0$   |

Table 2. The material density, band gap energy and resistivity of semiconductor materials

| Property        | Si     | GaAs   | 4H SiC | GaN   | AlN   | Diamond |
|-----------------|--------|--------|--------|-------|-------|---------|
| Density (g/cm$^3$) | 2.33   | 5.40   | 3.21   | 6.10  | 3.26  | 3.52    |
| Bandgap (eV)    | 1.1    | 1.43   | 3.26   | 3.45  | 6.2   | 5.45    |
| Resistivity (Ohm·cm) | 1000   | $<10^8$| $>10^{12}$| $>10^{10}$| $>10^{13}$| $>10^{13}$|

Figure 1. The basic mechanisms of conversion of radiation flux into electricity.
2. Physical model of a betavoltaic microbattery

The universal physical model of low-power betavoltaic microbatteries based on the commercial TCAD Synopsys Sentaurus platform was described in our work [13]. The model is suitable for I-V characteristics and a full set of parameters ($I_{sc}$, $V_{oc}$, $P_{max}$, $I_{dark}$, $\eta$) simulation of betavoltaic elements with different types of beta-emitting sources and different 2D/3D constructions of pn-junctions diodes fabricated on the basis of the different semiconductor materials: Si, SiC, Ge, GaAs.

The general model consists of two parts: a model for a radioactive source and a model for pn-junction diode structure.

Model of EHP generation. Beta particles, emitted from the radioactive source, pass through the pn-junction structure and generate EHPs by ionization and excitation with rate $G$. The generation rate $G$ as a function of the material depth was experimentally obtained in [11] for three semiconductors Si, Ge and SiC under Ni-63 irradiation. It is presented in Figure 3.

The photovoltaic analogy was used to receive the mathematical description of the experimental curve in Figure 3. It is known that for the photovoltaic diode in the one-dimensional approach the following function for $G(x)$ can be used:

$$G(x) = \phi_0 \alpha e^{-\alpha x},$$

Figure 2. Multi-sectional betavoltaic structure: a) microchannel section with deep trench isotope source; b) PN-junction current density vs microchannel width.
where: \( \Phi_0 = (1 - r) \cdot P / (Ahf) \) is the incident beta particle flux; \( P \) is the incident power converging on the junction; \( \alpha \) is the absorption coefficient of silicon; \( h \) is Plank’s constant \((6.626 \cdot 10^{-34} \text{ J}\cdot\text{s})\); \( f \) is the photon frequency; \( r \) is the electron backscatter coefficient; \( A \) is semiconductor chip surface area.

The obtained from Figure 3 values of the power \( P \) and wavelength \( \lambda \) of a visible light source that produces the same ionization effect for silicon as beta particle flux, are the following: \( P=4.33 \cdot 10^{-7} \text{ W/cm}^2 \) and \( \lambda=450 \text{ nm} \). These values are used as input data of the TCAD physical model for electrical I-V-characteristics simulation.

Model of pn-junction electrical behavior. The TCAD physical model is based on the classical set of equations for electrons and holes transport, Poisson equation for electro-static potential distribution, Shockley-Read–Holl and Auger surface and volume recombination rates \( R_s \) and \( R_v \). The continuity equations for electron and hole current densities \( j_n \) and \( j_p \) include the EHP generation rate \( G \) defined at the previous step in Eq. (1):

\[
\frac{\partial n}{\partial t} = G - (R_s + R_v) + \frac{1}{q} \nabla j_n , \quad \frac{\partial p}{\partial t} = G - (R_s + R_v) + \frac{1}{q} \nabla j_p ;
\]

(2)

Numerical solution of the classic set of physical equations for the semiconductor device structure is used in the TCAD Synopsys Sentaurus tool for I-V-characteristics simulation.

3. Simulation results

Two types of betavoltaic batteries with the most popular for practical applications Ni-63 emitting isotope source and N'-N-P' diode structure were investigated.

![Figure 4. Doping profiles for Device №1](image)

A. Device №1 with doping profiles (Figure 4) was examined at normal temperature \( T=300 \text{K} \). The simulated I-V- characteristics for ideal abrupt pn-junction is presented in Figure 5. The following parameters of the betavoltaic element were obtained: open-source voltage 0.125 V and maximum current density 0.24 nA/cm\(^2\). For comparison, analogous parameters from [11] are 0.11V and 0.23 nA/cm\(^2\), respectively. It is interesting to know the simulation error caused by ideal abrupt doping profile assumption. In Figure 6, two simulated curves for the parameter \( V_{oc} \) determination are presented for ideal abrupt and Gaussian doping profiles: for abrupt pn-junction \( V_{oc}=1.25 \text{V} \), for Gaussian \( V_{oc}=0.08 \text{V} \). The difference is too much for practical applications. This means that abrupt pn-junction approximation which was used in all the earlier published works, can be used only for qualitative analysis.

B. Device №2 with heavily doped N' Gaussian profile with \( N_s=10^{20} \text{ cm}^{-3} \), \( x_j=0.68 \mu\text{m} \) and lowly doped P-substrate with \( N_{sub}=10^{14} \text{ cm}^{-3} \) and \( W_{sub}=50 \mu\text{m} \) was investigated in the temperature range 213…303 K. The simulated curves for the temperatures 213 K, 263 K and 303 K are presented in Figure...
7. The simulated characteristics were compared with the experimental characteristics obtained for an analogous device [14] (Table 3). The qualitative agreement was achieved.

From the I-V-characteristics presented in Figure 7, the temperature dependencies of the parameters ($V_{oc}, J_{sc}, P_{max}, \eta$) for the betavoltaic microbattery based on the Device №2 were extracted (Figure 8(a) and Figure 8(b)).

The theoretical results presented in Figure 8 confirm the fact that the parameters $V_{oc}, P_{max},$ and $\eta$ are linearly growing with temperature reducing. The temperature dependencies are strong, and in the temperature interval 213…303 K the parameters are increased almost ten times. On the contrary, the parameter $J_{sc}$ is decreased slightly. This observation is attributed mainly to the increase in bandgap of semiconductor material with the decrease in temperature. Generally, this means that the efficiency of betavoltaic microbatteries is growing considerably at low temperature.

The simulated results in Figure 8 were compared with the theoretical and experimental results presented in [11, 14]. The good agreement was achieved. For example, in Table 4, the comparison of temperature sensitivity for the full set of simulated and measured parameters of the $^{63}$Ni-Si microbattery is presented.
Figure 8. Temperature dependencies of parameters $V_{oc}$, $J_{sc}$ (a) and $P_{max}$; $\eta$ (b) for betavoltaic microbattery based on the Device №2.

4. Conclusion
1. The universal physical TCAD model was adapted to $^{63}$Ni-Si betavoltaic microbattery characteristics simulation. The standard TCAD Synopsys Sentaurus optical generation model was adopted for simulation of electron-hole generation for beta particles irradiation.

2. The complete analysis of I-V characteristics and a set of basic parameters ($V_{oc}$, $J_{sc}$, $I_{dark}$, $P_{max}$, $\eta$) for betavoltaic silicon batteries under Nickel-63 irradiation in the temperature range 213-330 K was carried out using the universal physical TCAD model.

3. It was found that the main microbattery parameters ($V_{oc}$, $P_{max}$, $\eta$) are growing considerably at low temperatures, with the exception of the parameter $J_{sc}$, which decreases slightly when the temperature decreases. Thus, the fact that the efficiency of betavoltaic microbatteries is growing considerably at low temperature was confirmed.

4. The pn-junction diode energy converters with real Gaussian doping profiles were considered instead of devices with abrupt profiles. It was shown that abrupt pn-junction doping approximation causes considerable error in IV characteristics simulation and can be used only for qualitative analysis.

5. The simulated current-voltage characteristics of the $^{63}$Ni-Si betavoltaic elements are in good agreement with the measured characteristics in the temperature range 213-330 K.

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