Modeling of microporous silicon betaelectric converter with $^{63}$Ni plating in GEANT4 toolkit*

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Abstract. The model of electron-hole pairs generation rate distribution in semiconductor is needed to optimize the parameters of microporous silicon betaelectric converter, which uses $^{63}$Ni isotope radiation. By using Monte-Carlo methods of GEANT4 software with ultra-low energy electron physics models this distribution in silicon was calculated and approximated with exponential function. Optimal pore configuration was estimated.

Introduction

New generation micropower devices need compact and long-lifetime power supplies. One of perspective ways to create such devices is using Direct Conversion Nuclear Batteries based on the betavoltaic effect. Semiconductor betavoltaic converter of $^{63}$Ni isotope radiation investigated by multiple scientific researches. $^{63}$Ni isotope emits only beta-particles, without gamma and alpha radiation. Irradiation energy level below structural damage energy for most semiconductors and isotope half-decay time at about 100 years.

Isotope undergoes radioactive decay

$$^{63}_{28}\text{Ni} \rightarrow ^{63}_{29}\text{Cu} + e^-,$$

the result of which is emission of electron ($\beta$-particle) having average energy 17.3 keV with a random direction. During travel through the space-charge region of p-i-n junction such particle causes the generation of electron-hole pair (EHP) which is being separated by the built-in electric field. Separated charge carriers travel to the opposite directions: holes into the p-region, electrons into the n-region. As the result, difference of potentials is induced on p and n region leads, the same way as it occurs inside photoelectric converter. If connectors are attached to external resistance, the current flows through the circuit (e.g. micropower voltage regulator) and generated energy can be used to power the load.

The main advantages of radioisotope-based power sources are long service life (determined by half-decay time), high specific energy, high energy density, wide range of operational environment conditions (determined by semiconductor) and high reliability. It is possible to create flexible

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One of viable designs of beta-electrical converter (BEC) is silicon wafer with deep micropores, every pore of which is turned into p-i-n junction and plated with $^{63}$Ni. The main advantage of this design is significant increase of junction area and as the result – the increase of volumetric density of energy.

It is necessary to perform the modelling of all energetic processes – primary beta-electrons generation, electron-hole pairs generation, particles diffusion and drift inside space-charge region, recombination and others. It is possible to use COMSOL Multiphysics or Centaurus TCAD for modelling some of listed processes, but they do not incorporate the model of betavoltaic particles generation. For this reason Monte-Carlo method modelling using GEANT4 software was performed to estimate the distribution of EHP generation rate in semiconductor.

**Construction definition**

There are different possible designs of BEC: planar, microporous and microchannel with different geometrical parameters, microgranular designs are currently under development in modern scientific papers. The main aim of a switch from flat design to more advanced is to increase the junction area, because $^{63}$Ni isotope has limited specific surface activity as deep placed atoms’ radiation is shielded by surface atoms. $^{63}$Ni is completely artificial, thus its cost significantly exceeds the price of silicon BEC - it is necessary to work out the design having optimal amount of this isotope. As was found out in earlier research [4], the total EHP generation curve as a function of isotope thickness is approximated by the exponent $a \cdot \exp(-\Delta y/T_y)$, where $a = 0.1878$, $T_y = 0,7987 \mu m$. The layer having thickness of $3 \cdot T_y = 2,4 \mu m$ generates 95% of useful energy, further increment of thickness does not increase useful energy generation.

Isotope application onto microporous silicon can be performed in different ways, one of the most simple is electrochemical deposition. When this method is used, nickel is deposed not only onto the surface of the pores, but also onto the outer surface of converter. As electrons are emitted by the isotope into a random direction, half of outer surface sourced radiation would be lost. To capture this radiation, extra BEC can be used, microchannel or planar type. When microchannel one is used, its outer nickel layer would screen some part of bottom BEC’s radiation. Thus it becomes practical to use the planar BEC without isotope layer. In this case the design becomes hybrid as shown on figure 3(a), radiation of isotope is utilized in optimum way.

It is necessary to predict the optimum shape of microchannels on the basis of isotope surface layer area maximization and minimization of its volume.

The picture 2(a) shows the schematics of the oval microchannel, here $R$ - radius of circular
pore section, \( L \) - length of straight section, \( d \) - isotope layer thickness. Outer perimeter is estimated as \( L_{\text{perimeter}} = 2\pi R + 2L \), isotope surface area as \( S_{\text{Ni layer}} = \pi R^2 - \pi (R - d)^2 + 2Ld \). The isotope utilization efficiency is estimated as pore perimeter divided by isotope layer area:

\[
    k_{\text{eff}} = \frac{L_{\text{perimeter}}}{S_{\text{Ni layer}}} = \frac{2\pi R + 2L}{\pi R^2 - \pi (R - d)^2 + 2Ld}.
\]

Let us assume the isotope thickness \( d = 0.7\mu m \) and variate the values \( R \) and \( L \) in range, acceptable within current technology for microchannel manufacturing. Calculation results \( k_{\text{eff}}(R, L) \) are shown on figure 2(b). One can see, that the extremal point lays near the minimum values of \( R \) and \( L \). It is possible to conclude, that the most efficient shape is cylindrical pores.

![Figure 2.](image)

Figure 2. a) micropore geometry; b) plot of \( k_{\text{eff}}(R, L) \) function; c) cellular micropore structure.

Circular microchannels should be placed on the surface of silicon wafer due to criteria of maximum surface utilization. As the pore is symmetrical along its longitudinal axis, the zone of carrier generation along the pore would be symmetrical as well. The maximum surface would be achieved when honeycomb placement is used, as shown on figure 2(c).

### Computational problem definition

Current article propose to use the electron-matter interaction model, defined for low levels of energy. For instance, model proposed in [2] describe the ionization and electron transition into conduction zone for energy range from 16.6 eV to 50 keV. The calculated interaction cross-sections are used to plot the tracks of beta-electrons for isotope \(^{63}\text{Ni} \) in silicon.

The selected geometrical schematic of this problem is shown on figure 3(a). The object is a cuboid, consisting of several parts: two silicon beta-electrical converter (BEC) of planar and micropore types, coated with layer of isotope Ni63, and air gap between BECs. Air also fills free space inside pore. Size of ”World” region is 120\( \mu m \) in x and y dimensions. Planar BEC have thickness of 40\( \mu m \), micropore BEC – 140\( \mu m \). Pore diameter is 20\( \mu m \), depth is 100\( \mu m \). In conformity with article [1], economically efficient width of isotope layer taken 0.7\( \mu m \).

Fast electrons generation takes place in the isotope layer. The spectrum of beta-radiation corresponds to \(^{63}\text{Ni} \) isotope (from [1]), approximated with exponential function \( a \exp(-b \cdot E) \), where \( b = 50.09 \text{ MeV}^{-1} \) (from [4]).

Particle tracks start from the isotope layer. Figure 3(b) shows the resulting beta-electrons tracks in silicon in cylindrical coordinate system \((r, \varphi, z)\), averaged along the axis \( \varphi \).
Calculation sequence:

(i) Tracks calculation in GEANT4, corresponding to the software-defined experiment schematic;

(ii) Saving tracks data (nodal points coordinates, the amount and type of energy loss) as CSV-files;

(iii) Reading of generated CSV-files into memory, saving to float data files;

(iv) Separation the data of every track from whole data array, taking in consideration only ionization losses; secondary electrons are filtered out from tracks data, they are taken into account as separate particle tracks);

(v) Ionization energy losses (the number of electron-hole pairs generated) is calculated for every elementary volume of silicon.

(vi) Calculation of electron-hole pairs generation rate field in semiconductor.

The most informative in terms of p-i-n junction parameters optimization is middle, base part of micropore marked with red rectangle at 3(b).

Results and discussion

Representative segment of field was separated, and estimated field of energy generation rate was normalized relative to total initial energy of beta-radiation:

\[
E_{\text{norm}} = \frac{1}{E_{\text{total}}} \frac{S_{\text{pore side area}}}{S_{\text{total Ni63 layer}}} \sum_{z} \sum_{\varphi} E(r, \varphi, z).
\]

where \(E_{\text{total}}\) – total radiated energy, eV; \(S_{\text{pore side area}}\) – pore surface area, taking part in the calculation; \(S_{\text{total Ni63 layer}}\) – total isotope layer area; \(r, \varphi, z\) – coordinates of cylindrical coordinate system.
Normalized field of energy generation rate (one-dimensional normal to surface, pointed into the depth of semiconductor) was approximated using exponential function \[5\], translated at 4.

Figures 4 and 3(b) represent the modelling results. The main modelling conclusions are: the beta-electron flow increase takes place near the corners, air gap of 1um does not shield beta-electron flow.

GEANT4 source code used for track estimation is uploaded to GitHub*. Number of tracks used for simulation was 40000, to increase the simulation precision. Calculation was separated into 4 threads to minimize the simulation time.

![Figure 4](image)

**Figure 4.** Normalized energy field of carrier generation, a) 3D; b) 1D field.

**Conclusion**

As a result of the performed research it is revealed that

a) Minimum distance between micropores should be at least 20\(\mu m\). It is defined by maximum beta-electron energy. Maximum distance can be limited by the decline in silicon utilization efficiency. Optimum distance is more than 20\(\mu m\).

b) Micropore depth should be maximized and its diameter - minimized within limits of used technology for micropore creation and isotope plating. The shape should be as close to cylindrical as possible.

c) The highest generation rate density is near the open end of micropore. P-i-n junction quality should be the highest possible in this area to minimize parasitic currents.

d) The field of EHP generation rate was estimated, so that it is possible to optimize parameters of silicon semiconductor structure. Calculated exponential function approximation parameters can be used to define the fields for numeric modelling of beta-electrical converters, in software like Comsol Multiphysics.

**References**

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