Postprint: Carrier-Evolution-Based 3D P+PNN+ Multi-Trench Structure for Enhanced Betavoltaic Nuclear Battery Performance

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Date: 2024-02-01T00:00:00+00:00

Abstract

Betavoltaic nuclear batteries, which utilize beta particles emitted by radioactive isotopes to achieve electrical energy conversion, are widely regarded as a highly promising alternative energy technology. To meet the power requirements of microelectromechanical systems (MEMS), researchers have proposed employing three-dimensional (3D) structures as a potential solution. In this context, this study introduces a novel 3D battery design featuring a P+PNN+ multi-trench structure based on 63Ni-SiC material. This structure is unique in that it eliminates the need for epitaxial PN junctions on the inner surfaces of trenches in semiconductor devices, thereby reducing leakage current and power loss. Through the Monte Carlo simulation method with comprehensive consideration of a fully coupled physical model, we successfully extended the electron-hole pair generation rate (G(x)) to 3D structures, enabling the efficient design and development of betavoltaic batteries with complex 3D architectures. The results demonstrate that, compared with conventional planar batteries, our proposed 3D battery achieves a superior maximum output power density of 19.74 $\mu W/cm^2$, with corresponding short-circuit current, open-circuit voltage, and conversion efficiency of 8.57 $\mu A/cm^2$, 2.45 V, and 4.58%, respectively. Furthermore, we utilized COMSOL Multiphysics software to conduct an in-depth analysis of charge carrier transport and collection characteristics, providing profound insights into the mechanism of battery output power enhancement and elucidating the discrepancies between ideal and simulated performance of betavoltaic batteries. This study furnishes a forward-looking methodology for the design and optimization of high-output-performance betavoltaic nuclear batteries, while also offering valuable references for future battery device fabrication.

Full Text

ABSTRACT

Betavoltaic nuclear batteries offer a promising alternative energy source that harnesses the power of beta particles emitted by radioisotopes. To satisfy the power demands of microelectromechanical systems (MEMS), three-dimensional (3D) structures have been proposed as a potential solution. Accordingly, this paper introduces a novel 3D 63Ni-SiC-based P+PNN+ structure with a multi-groove design that avoids the need for PN junctions on the inner surface, thereby reducing leakage current and power losses.

Monte Carlo simulations were performed using a fully coupled physical model to extend the electron–hole pair generation rate to a 3D structure, enabling the efficient design and development of betavoltaic batteries with complex geometries. The proposed model achieves a significantly higher maximum output power density of 19.74 μW/cm^2, with corresponding short-circuit current, open-circuit voltage, and conversion efficiency of 8.57 μA/cm^2, 2.45 V, and 4.58%, respectively, compared with conventional planar batteries. Through analysis of carrier transport and collection characteristics using COMSOL Multiphysics, we provide deep insights regarding power enhancement and elucidate the discrepancies between ideal and simulated performances of betavoltaic batteries. Our work offers a promising approach for the design and optimization of high-output betavoltaic nuclear batteries with a unique 3D architecture and serves as a valuable reference for future device fabrication.

Keywords: Betavoltaic nuclear battery; High-output power density; Three-dimensional structure; Carrier drift-diffusion; Carrier recombination; Carrier collection efficiency.

1. INTRODUCTION

Microelectromechanical systems (MEMS) have attracted tremendous interest for various applications ranging from mobile electronics to deep-sea surveys, implantable medical devices, and autonomous wireless sensor networks, owing to their remarkable performance, compact size, and suitability for high-volume production. However, the development of micro-batteries capable of delivering 1–100 W of power, providing long service life, and fitting within the size range of 1 m to 10 mm has become a critical challenge for MEMS applications [**?**]. Recently, betavoltaic nuclear batteries have emerged as a highly attractive energy option for MEMS applications, offering potential advantages including long operational life, high energy density, ultra-miniature size, and strong anti-interference capability [**?**].

The performance of betavoltaic nuclear batteries is governed by radioisotope source characteristics, device geometry, and semiconductor converter properties. The corresponding relationship can be mathematically expressed as:

$$P_m = AE_{avg}\eta_s(1-r)\eta_c = AE_{avg}\eta_s(1-r)QV_{OC}FF$$

where A is the radioisotope activity determined by the radioisotope half-life, E_{avg} is the average β-decay energy dictating the total input power driving the converter, η_s is the fraction of β-energy emitted relative to the total decay energy of the radioisotope source, r is the reflectivity coefficient, η_c is the energy conversion efficiency of the semiconductor converter, Q is the carrier collection efficiency, V_{OC} is the open-circuit voltage, FF is the fill factor, and ε is the effective ionization energy to generate an electron–hole pair (EHP). The overall conversion efficiency can be expressed as: $\eta_{tot} = \eta_s(1-r)\eta_c$. The output power of betavoltaic nuclear batteries depends on significant losses, such as self-absorption loss $(1-\eta_s)$ in the radioisotope source, backscattering loss (r) at the semiconductor interface, and carrier collection loss $(1-Q)$ outside the depletion region [**?**]. To maximize energy coupling between the radioisotope and semiconductor, it is crucial to increase their face-to-face area while reducing self-absorption and backscattering effects. Additionally, η_c depends on material properties of the semiconductor, including bandgap, depletion region width, and carrier diffusion length. The parameters Q, V_{OC}, and FF can be improved through optimization of doping concentrations and junction width to increase the depletion region width and carrier diffusion length, ensuring that the β-particle penetration depth matches the converter scale length.

The conventional planar configuration of betavoltaic nuclear batteries uses only one side of the radioisotope source attached to the semiconductor converter, which limits output power and conversion efficiency. A high activity (A) or input power (P_{in}) requires a thick source layer, but this results in stronger self-absorption effects and smaller η_s, saturating $A \cdot \eta_s$. The directional loss is approximately 50%, and backscattered loss significantly reduces device efficiency by up to 25% [**?**, **?**]. Although efforts have been made to improve conversion efficiency and output power—including using a reflector to reduce directional and backscattered losses [**?**], optimizing junction depth and doping concentration to increase carrier collection efficiency [**?**], employing an extra graded N-layer to reduce radiation-induced EHP recombination loss [**?**], and adopting radioisotope sources with higher particle energy to increase input power [**?**]—reported values remain limited by the effective loading activity of the radioisotope source and the coupling efficiency between source and device, i.e., the limitation of $A\eta_s(1-r)$. Consequently, practical and tested batteries achieve only 0.1–50 nW output power [**?**], while theoretically predicted ones reach 10–400 nW [**?**, **?**, **?**, **?**], falling short of MEMS power requirements [**?**].

To achieve higher performance in betavoltaic nuclear batteries, $A\eta_s(1-r)$ can be increased over a wide range using specific radioisotope sources and semiconductor materials. Increasing the specific surface area of the converter enables higher loading of radioisotope sources, leading to larger $A\eta_s(1-r)$ and higher output power. Compared with two-dimensional (2D) planar structures, three-dimensional (3D) structures with larger specific surface area can significantly increase output power density through three mechanisms: (i) more radioisotope sources can fill the interspace of 3D structures, (ii) thinning of radioisotope sources in 3D structures significantly reduces self-absorption effects, and (iii)

combination of a radioisotope source with 3D structures enables beta particle interaction with the converter in all directions, increasing beta particle collection efficiency.

In recent years, 3D structures in betavoltaic nuclear batteries have demonstrated significant potential for improving specific surface area and conversion efficiency, making them promising options for meeting MEMS power demands [**?**]. However, conventional 3D structures require preparation of PN or PIN junctions on the inner surface of the microstructure, which significantly affects leakage current and output performance [**?**]. This is a predominant reason why device performance remains far from ideal, sometimes by several orders of magnitude, making full utilization of the 3D structure challenging. Moreover, while Monte Carlo simulations [**?**, **?**] and empirical formulas [**?**, **?**] are widely employed to calculate the EHP generation rate distribution [$G(x)$] in betavoltaic nuclear batteries with 2D diode structures, the EHP generation rate is rarely evaluated in 3D structured converters combined with radioisotope sources distributed in 3D space. Most currently available models for $G(x)$ in 3D structured converters only describe specific structures with fixed source and device geometries and cannot accurately evaluate EHP distribution in 3D structures, highlighting the need for a precise model to advance 3D battery development.

This paper introduces a novel approach that addresses these issues by utilizing a 63Ni-SiC-based (P+PNN+) structure with a multi-groove design, enabling epitaxial growth of graded P and N layers on the substrate without preparing PN junctions on the inner surface of the microstructure. This approach has the potential to significantly reduce leakage current and power losses, thereby narrowing the gap between theoretical predictions and experimental results. In addition, a novel formulaic model is proposed for calculating the complex EHP generation rate in 3D-structured betavoltaic nuclear batteries. The model considers the intricate 3D structure of the converter and radioisotope source, enabling accurate evaluation of EHP distribution in all possible 3D structures resulting from geometry changes. Our fully coupled model, combined with COMSOL Multiphysics, encompasses the entire physical process of carrier evolution, including β-particle generation, energy deposition, radiation-carrier generation, drift-diffusion, and recombination. This study provides valuable insight into the internal mechanisms of carrier transport, collection characteristics, and power enhancement. Our approach demonstrates maximized output power density with optimized source thickness, converter geometry, doping concentration, and width of each region, outperforming conventional planar batteries. The novel $G(x)$ model provides a critical tool for designing and optimizing 3D structured betavoltaic nuclear batteries, with potential applications in other betavoltaic systems.

2.1 Device Structure

Figure 1: see original paper depicts a 63Ni-SiC-based betavoltaic nuclear battery with a multi-groove structure, characterized by ridge width [d], ridge spacing

[t], and groove depth [H_{source}]. The converter comprises four layers: a P+-SiC layer, graded P-SiC layer, graded N-SiC layer, and N+-SiC layer with thicknesses of H_{P+}, H_P, H_N, H_{N+} (the N+-layer thickness is slightly larger than H_{N+}), respectively. The 63Ni source fills the multi-grooves, surrounded by converters at the sides and bottom (front and rear sides not shown), and enclosed by a metal electrode at the top. This design reduces directional and electrode shielding losses compared with conventional planar diode structures. The rectangular top section of the device has an area of 1 cm × 1 cm. To prevent PN junction shorting and metal-semiconductor contact formation, techniques such as nitride passivation, plasma-enhanced chemical vapor deposition, and atomic layer deposition can be employed to grow a thin insulating layer (e.g., Si_3N_4, SiO_2, and Al_2O_3) with a thickness of 10–100 nm [**?**]. This layer effectively blocks the flow of electrons or holes, achieving insulation between the source and semiconductor devices while having negligible impact on energy deposition of the source decay energy in the device.

To ensure good Ohmic contact, the doping concentrations of heavily doped P+-SiC and N+-SiC layers are 10^{19} and 10^{18} cm^{-3}, respectively. The P- and N-SiC layers serve as the core regions of the betavoltaic nuclear battery, generating an internal electric field to separate radiation-induced EHPs. These layers are lightly doped to obtain larger depletion region width [W_d] and minority diffusion length [L_n or L_p], promoting EHP collection, as depicted in Fig. 1(b). The gradient interface between the P+/P and N/N+ layers generates an extra electric field that reduces surface recombination and enhances EHP collection. In this 3D structure, EHPs are mainly generated in the ridges, and these areas contribute most to the output power. Monte Carlo simulations and COMSOL Multiphysics were used to optimize structural parameters, including the thickness of each doping region, doping concentration, ridge width, and ridge spacing, and to predict battery output performance. The 63Ni source was selected as the beta source due to its long half-life (approximately 100 years), moderate decay energy ($E_{avg} = 17.4$ keV, $E_{max} = 66.9$ keV), and solid metal form, which allows easier and safer handling. SiC was selected as the converter semiconductor material because of its desirable properties including low leakage current density, higher radiation damage threshold, higher conversion efficiency, and excellent tolerance to harsh environments such as extreme temperatures, wear, chemical exposure, and radiation [**?**]. Moreover, the development of SiC etching technology has enabled fabrication of microgroove structures with high aspect ratio [**?**].

2.2 Methods

2.2.1 Radiation-Induced Carrier Generation in 3D Diode Structures

A. Model for Radiation-Induced Carrier Generation Rate in 3D Diode Structures The distribution of the EHP generation rate in a betavoltaic nuclear battery is governed by the energy deposition of beta particles in the converter, which significantly affects output performance. In the conventional pla-

nar diode structure depicted in Fig. 2 Figure 2: see original paper, the energy deposition $[E_{dep}(x)]$ along the radiation transport depth $[x]$ in bulk SiC was calculated via Monte Carlo simulation with the Geant4 radiation transport toolkit, using a rectangular 63Ni source with a full energy spectrum. The 63Ni source is characterized by a specific activity of 5.68 Ci/g, 100% abundance, and density of 8.9 g/cm^3, with isotropic emission of beta particles. SiC has a bandgap width of 3.26 eV, relative dielectric constant of 9.7, density of 3.21 g/cm^3, and intrinsic carrier concentration of 7.4×10^{-9} cm^{-3}, derived using a widely employed formula [**?**]. $G(x)$ is obtained and expressed as:

$$G(x) = A \cdot E_{dep}(x) = G_0 \exp(-\alpha x)$$

where A is the activity of the radioisotope, ε is the average energy needed to generate an EHP (commonly considered as 6.88 eV for SiC [**?**]), and G_0 and α are the surface EHP generation rate and absorption coefficient, respectively. $G(x)$ for 63Ni sources with varying thickness $[t]$ is presented in Fig. 2(c), and the corresponding G_0 and α are derived by fitting $G(x)$. The dependences of G_0 and α on source thickness $[t]$ are then fitted, as demonstrated in Fig. 2(d). Consequently, $G(x)$ considering different source thicknesses is expressed as:

$$G(x,t) = A_1(1 - e^{-\mu_1 t})e^{-(A_2 e^{-\mu_2 t} + B_2)x}$$

with fitting parameters provided in Table 1 . Fig. 2(c) shows that the saturation thickness of the 63Ni source is 3 m, consistent with previous work [**?**, **?**]. The penetration depth of β particles emitted from 63Ni is 10.2 m in SiC, defined as the location where 99% of the total energy deposition occurs according to Alam [**?**].

To accurately model energy deposition and EHP generation rate in a multi-groove betavoltaic nuclear battery, it is essential to consider superposition contributions from all isotope sources and ridges. This involves extending $G(x,t)$ from the 2D structure to the 3D structure. Fig. 2(a) characterizes the penetration distance distribution of β particles released by 63Ni isotope sources, where D_j denotes the jth layer converter (the jth ridge of the proposed battery) and S_j indicates the jth 63Ni layer. At a random location where EHPs are generated in converter D_j (specified by reference site P), the distance between P and source S_{j-1} is represented by $[x]$. Converter D_j is exposed to $[j-1]$ layers of isotope sources on its left, and β particles emitted from the ith $(i < j)$ source must traverse a total source thickness of $[(j-i-1)t]$ and a total converter thickness of $[(j-i-1)d+x]$ to reach reference site P. Similarly, D_j is exposed to $[n+1-j]$ layers of sources on its right, and β particles emitted from the kth $(j \le k \le n)$ source must penetrate a total source thickness of $[(k-j)t]$ and a total converter thickness of $[(k+1-j)d-x]$ to reach P. During this process, the energy of beta particles decays exponentially with penetration distance, and the EHP generation rate of D_j is given by:

$$G_j(x,t) = \sum_{i=j-1} \{G_0(t)e^{-\alpha(t)((j-i-1)d+x)}e^{-\gamma(t)(j-i-1)t}\} + \sum \{G_0(t)e^{-\alpha(t)((k+1-j)d-x)}e^{-\gamma(t)(k-j)t}\}$$

where n is the number of source layers, $G_0(t)$ is the surface EHP generation rate, $\alpha(t)$ is the absorption coefficient of β-electron flux in SiC, and $\gamma(t)$ is the absorption coefficient of β-electron flux in 63Ni, acquired via the equation in Table 1 based on Monte Carlo code simulation. The EHP generation rate of the $(n+1)$th converter can be expressed as $G_{n+1}(x,t) = G_1(d-x,t)$, owing to symmetry of the multi-groove structure. Table 1 shows that the R^2 (R-squared or coefficient of determination) values are greater than 0.99, indicating excellent fitting performance of the model.

B. Validation of Electron-Hole Pair Generation Rate Model in 3D Diode Structures Accurate prediction of the EHP generation rate is essential for optimizing the design of 3D SiC-based betavoltaic nuclear batteries. Therefore, the validity and predictive capability of the model were demonstrated through comparison with original Geant4 data $[AE_{dep}(x)/\varepsilon]$. Figs. 2(e)-(g) exhibit the reliability of the proposed EHP generation rate model, expressed by formula (3), with highly consistent $G(x,t)$ curves compared with original Geant4 data for ridge spacings of 1.5 and 1 m, and ridge widths of 3 and 4 m. The high R^2 values of 0.985, 0.990, and 0.982 for these curves indicate the accuracy of the model in calculating EHP generation rates in 3D structures, rendering it a valuable tool for optimizing SiC-based betavoltaic nuclear batteries for high performance.

In the 2D converter, the EHP generation rate decreased exponentially with depth, whereas the multi-groove 3D structure exhibits a unique distribution of higher EHP generation rates in the inner ridges and lower rates in the outermost ridges. The innermost ridges exhibit high EHP generation rates on the lateral surfaces, low rates in the middle, and a symmetrical distribution, matching the 3D EHP distribution in the inner ridge shown in Fig. 1(a). These findings suggest that the proposed multi-groove 3D structure has the potential to significantly enhance power output compared with traditional 2D structures, particularly as relative depth increases.

2.2.2 Model for Radiation-Induced Current in 3D Diode Structures

Fig. 1(b) illustrates that radiation-induced EHPs generated within the depletion region can be collected with 100% efficiency, whereas those generated outside the depletion region can only be collected after diffusion to the PN junction boundary, the P+/P interface, or the N/N+ interface. The collection efficiency $CE(y)$ was calculated using the equation [**?**]:

$$CE(y) = 1 - \tanh\left(\frac{d(y)}{L}\right)$$

where $d(y)$ represents the distance from the depletion region boundary or the interfaces and is set to zero inside the depletion region. The electron and hole minority carrier diffusion lengths L are expressed as L_{n1}, L_n, L_p, and L_{p1} in

regions P+, P, N, and N+, respectively. The radiation-induced current density J_R can be expressed as:

$$J_R = \left(\sum_{i=n+1} q \int G_j(x,t) H_{source} CE(y) dy \int dz \right)$$

where q is the electron charge; H_1 is the ridge width $[d]$; and H_2 and S are the rectangular side length (1 cm) and area of the device (1 cm^2), respectively.

According to drift-diffusion theory, nonequilibrium carriers generated within the depletion region and the neutral region outside the depletion region boundary within a minority diffusion length can be collected, thus contributing to the current density (J_R). The effective charge collection region (ECR) length, represented by $H_{ECR} = (W_d + L_{n1} + 2L_n + 2L_p + L_{p1})$, determines J_R and can be maximized by increasing W_d, L_{n1}, L_n, L_p, and L_{p1}. Lower doping concentrations increase W_d and L, leading to higher EHP collection, as demonstrated in Figs. 3(a) and (b), where W_d decreases from 7.58 m to 30 nm and L_n decreases rapidly from 77.34 to 11.06 m with increasing doping concentration from 10^{14} to 10^{19} cm^{-3}. L_p decreases more gradually over the same doping range. The minimum doping concentration in the P- and N-regions was 10^{14} cm^{-3} due to our facility' s capacity to process low doping in SiC materials, whereas the minimum doping concentration of the heavily doped P+- and N+-regions required $N_A = 10^{19}$ cm^{-3} and $N_D = 10^{18}$ cm^{-3}, respectively, to reduce ohmic contact resistance. To maximize H_{ECR} and J_R, the maximum values of W_d, L_{n1}, L_n, L_p, and L_{p1} should be adopted, as listed in Table 2 and detailed in Supplementary Materials S1 and S2.

2.2.3 Battery Output Characteristic Model and Simulation

The electron (hole) concentration $[n(p)]$ inside the semiconductor converter device is governed by the carrier continuity equation as follows:

$$\nabla \cdot j_n + G - R_n$$

$$\nabla \cdot j_p + G - R_p$$

where j_n (j_p) is the electron (hole) current density, G is the EHP generation rate derived from Eq. (3), and R_n (R_p) is the electron (hole) recombination rate. The current densities can be described by drift and diffusion processes [**?**] as:

$$j_n = nq\mu_n E + qD_n \nabla n$$

$$j_p = pq\mu_p E - qD_p \nabla p$$

where E is the sum of the external and internal electric fields generated by EHP diffusion. These relationships are governed by the Poisson equation:

$$\nabla \cdot (\epsilon_0 \epsilon_r \nabla V) = -q(N_D - N_A + p - n)$$

where ρ is the charge density, ϵ_0 is the vacuum permittivity, ϵ_r is the relative permittivity of the semiconductor, and N_D (N_A) is the donor (acceptor) concentration.

A. Current-Voltage Characteristics of Ideal PN Junction Diodes The current-voltage (J-V) characteristics of an ideal long PN junction diode can be derived assuming that the external voltage drops entirely in the depletion region, the diode operates under low injection level (i.e., the excess carrier concentration is much smaller than the equilibrium majority carrier concentration), there is no recombination or generation current in the space-charge region, the semiconductor is nondegenerate, and the length of the P- (N-) region is much larger than the diffusion length [**?**, **?**]. Under these assumptions, the J-V relationship of the neutral areas ($E = 0$) of the P- and N-regions can be obtained by solving the continuity equations (6)-(7) and current equations (8)-(9). Ignoring recombination and generation currents in the space-charge region, the J-V characteristics of an ideal diode are given by:

$$J = J_{SC} - (J_P + J_N) = J_{SC} - J_0 \left[\exp\left(\frac{qV}{kT}\right) - 1\right]$$

where J_{SC} is the short-circuit current, equal to radiation-induced current J_R; k is Boltzmann' s constant; T is the absolute temperature (300 K in this work); V is the bias voltage; and J_0 is the leakage current density of the PN junction. The open-circuit voltage is derived by setting $J = 0$:

$$V_{OC} = \frac{kT}{q} \ln\left(\frac{J_{SC}}{J_0} + 1\right)$$

The maximum output power P_m can be described as:

$$P_m = J_{SC} V_{OC} FF$$

where FF is the fill factor, which can be derived using the open-circuit voltage [**?**]. J_0 is determined by the diffusion efficiency and diffusion length of minority carriers and the doping concentrations, as shown in S3 of the Supplementary Materials. Using this ideal diode model, battery performance can be predicted quickly, and the optimal battery structure can be determined based on the J-V characteristic numerical model.

B. Current-Voltage Characteristics Calculation Using COMSOL Multiphysics The J-V characteristics of real diodes differ from those of ideal diodes due to various assumptions made for ideal PN junction diodes. Therefore, an accurate method is essential to simulate the J-V characteristics of real diodes, considering generation, recombination, and drift of charge carriers, as well as real characteristics of the semiconductor material. COMSOL Multiphysics is a powerful tool for simulating current-voltage characteristics under realistic conditions by solving partial differential equations that incorporate actual physical phenomena. The simulation utilizes various physical models, including Monte Carlo simulation for calculating the EHP generation rate in 3D diode structures (Equation (3)), the Shockley-Read-Hall model for trap-assisted recombination (Equation (14)) [**?**], and the low-field mobility model for determining minority

carrier mobility (Equations S4-S5 in the Supplementary Materials). Additionally, the carrier lifetime model is described in Equations S6-S7 in the Supplementary Materials:

$$R_{SRH} = \frac{C_p C_n N_t (np - n_i^2)}{C_n(n + n_i \exp((E_t - E_i)/kT)) + C_p(p + n_i \exp((E_i - E_t)/kT))}$$

$$R_{Auger} = (C_n n + C_p p)(np - n_i^2)$$
$$\tau_p(n + n_i \exp((E_t - E_i)/kT)) + \tau_n(p + n_i \exp((E_i - E_t)/kT))$$

Here, C_n (C_p) is the electron (hole) capture coefficient, n_i is the intrinsic carrier concentration, τ_n (τ_p) is the electron (hole) minority lifetime given by Equations S6-S7 of the Supplementary Material, E_t is the recombination center (defect) level, and E_i is the intrinsic Fermi level. The defect energy level is set as $E_t = E_i$, and the defect density is $N_t = 10^{13}$ cm^{-3}. Solving partial differential equations (6)-(10) yields important information on the electric field, carrier recombination, and electron (hole) current density, enabling prediction of crucial electrical parameters including short-circuit current [J_{SC}], open-circuit voltage [V_{OC}], and output power [P_m]. Ultimately, this approach accurately models diode behavior, which is vital for optimizing performance and ensuring that devices meet the requirements of various real-world applications.

3.1 Performance Calculated Using Ideal Diode Model

To optimize the structure of the proposed battery and maximize its output power density, a parametric sweep was conducted in the numerical model to adjust variables including single-source thickness (ridge spacing, t), single-converter thickness (ridge width, d), thicknesses of the P+-, P-, N-, and N+-regions (H_{P+}, H_P, H_N, and H_{N+}), acceptor concentration of P-region (N_a), and donor concentration of N-region (N_d). Possible values of t and d range from 0.1-10 m with a 0.1 m step size. It is worth noting that the source thickness is fixed to the saturation thickness of 3 m when t exceeds 6 m, and is evenly distributed on the inner surface of the microgroove. The feasible ranges for H_P and H_N are 1-250 m and 1-60 m, respectively, while N_a and N_d can range from 1×10^{14} to 7.94×10^{18} cm^{-3} and 1×10^{14} to 7.94×10^{17} cm^{-3}, respectively. The values for H_{P+} and H_{N+} are 10 and 6 m, respectively, which are close to the minority carrier diffusion length in the P+-region and N+-region. Additionally, the heavily doped P+-region and N+-region are assigned acceptor and donor concentration values of 1×10^{19} and 1×10^{18} cm^{-3}, respectively.

3.1.1 Optimizing Ridge Spacing and Width

The output power of a betavoltaic nuclear battery depends on the amount of beta particle energy deposited in the converters and the efficient collection of radiation-induced EHPs. The coupling between the radiation source and device is crucial for enhancing output power. To illustrate the impacts of t and d

on battery performance, 3D surface contours of short-circuit current density (J_{SC}), open-circuit voltage (V_{OC}), and maximum output power density (P_m) were plotted, as shown in Fig. 4 [Figure 4: see original paper].

As depicted in the 3D surface wireframe perpendicular to the d direction in Fig. 4(a), J_{SC} initially increases rapidly but subsequently decreases as t increases, reaching a peak value with t of 0.1–2.2 m. Additionally, the dependence of J_{SC} on d exhibits a similar trend, reaching its peak with d of 0.2–4.0 m. The bottom-projected contour shows that optimal J_{SC} values are achieved when d is in the range of 0.2–3 m and t ranges from 0.1 to 2 m. The maximum J_{SC} of 8.57 A/cm^2 is achieved by combining $t = 0.8$ m and $d = 1.2$ m.

Fig. 4(b) demonstrates that V_{OC} initially increases as t increases and reaches saturation at $t = 2$ m, while it decreases with increasing d. Nevertheless, V_{OC} is not highly sensitive to variations in t and d, with a range of 2.36–2.46 V. Due to minor variation in V_{OC}, P_m is primarily determined by J_{SC}. The relationship between P_m and variations in t and d exhibits a trend similar to J_{SC}, with rapid initial increase and subsequent slow decrease with increasing t or d, as illustrated in Fig. 4(c). The maximum P_m value of 19.73 W/cm^2 is attained at $t = 0.8$ m and $d = 1.2$ m.

The factors affecting output power mainly include A, η_s, $(1-r)$, Q, V_{OC}, and FF. With varying t and d, A, η_s, $(1-r)$, V_{OC}, and FF exhibit relative increases of 9844.28%, 578.19%, 1956.94%, 4.14%, and 0.21%, respectively, while Q remains unchanged at 45.64%. Therefore, the key factor affecting output power is the coupling of A, η_s, and r. For detailed calculations, please refer to Supplementary Material S4.

The input power [P_{in}] can be calculated by combining A, η_s, and r, as $P_{in} = AE_{avg}\eta_s(1-r)$. Figs. 4(d)-(e) present the maximum output power [P_m] and its corresponding optimized ridge width [d] of 0.2–4.0 m for different source thicknesses [t]. We found that P_m is determined by the coupling of A, η_s, and r, i.e., P_{in}. The optimized value of d gradually saturates with increasing t, consistent with the phenomenon of energy deposition saturation in the converter with increasing d. Additionally, the overall conversion efficiency [η_{tot}] increases and then decreases with t, reaching a saturated value of approximately 1.5%, and η_{tot} corresponding to maximum P_{in} and P_m is 4.58%.

In the proposed battery, smaller ridge spacing and ridge width can improve source activity and reduce self-absorption effect. However, excessively thin converters may result in lower $(1-r)$ and do not match the particle penetration depth, leading to reduced P_{in}. Therefore, a tradeoff between t and d is necessary to maximize power density.

3.1.2 Optimizing Widths of P-Region and N-Region

After optimizing t and d, we investigated the dependence of J_{SC}, V_{OC}, and P_m on the widths of the P- and N-regions, as shown in Figs. 5(a)-(c). Increasing

H_P results in an initial increase and subsequent saturation of J_{SC}, V_{OC}, and P_m. This trend can be attributed to increased radioisotope source activity with H_P, which generates more EHPs in the ECR. However, when H_P exceeds the ECR length, the performance metrics reach saturation. Specifically, J_{SC}, V_{OC}, and P_m saturate when H_P reaches 160 m, and an additional increase of 10 m results in a negligible increase of less than 1%. Similarly, J_{SC}, V_{OC}, and P_m present a comparable trend with H_N, showing gradual rise and saturation at $H_N = 24$ m. This phenomenon can be attributed to the longer minority carrier diffusion length ($L_n = 77.34$ m) of the P-region compared with that of the N-region ($L_p = 11.44$ m), and their saturation values of H_P and H_N are approximately twice L_n and L_p, respectively. Therefore, H_{source} should not exceed 200 m, where H_{P+} and H_{N+} are 6 and 10 m, respectively, and H_P and H_N should not exceed their saturation values of 160 and 24 m.

Fig. 5(d) shows that A linearly increases with H_P from 0.51 to 6.59 Ci (by 1204.00%), while Q first increases and then decreases with a relative change rate of 164.92%. The optimization of H_P reveals that factor A is the dominant factor affecting output power, and factor Q is secondary. Although A and Q show different trends with changes in H_P, their products, $A \cdot Q$ and P_m, exhibit consistent trends, further confirming that A and Q are the key factors affecting P_m, as shown in Fig. 5(e). However, V_{OC} and FF increase minimally by 1.81% and 0.09%, while η_s and $(1 - r)$ remain unchanged at 61.53% and 48.77%, respectively. Please refer to Supplementary Material S4 for detailed calculations.

As depicted in Fig. 5(f), for the structure with $H_{source} = 200$ m, J_{SC} and P_m initially increase with H_P and then decline instead of continuously increasing. This behavior occurs because the contribution of H_N to J_{SC} and P_m outweighs that of H_P when H_P approaches its saturation thickness. Therefore, when optimizing the widths of the P- and N-regions, the balance between H_P and H_N should be considered, as the combination of $H_P = 156$ m and $H_N = 28$ m achieves the maximum P_m of 19.74 W/cm^2. A longer P-region is more suitable for a betavoltaic nuclear battery with a P+PNN+ junction structure because it is more conducive to enhancing EHP collection owing to larger minority carrier lifetime and mobility compared with the N-region, as shown in Fig. S2 in the Supplementary Material.

3.1.3 Optimizing Doping Concentration in P- and N-Regions

Based on the analysis in Section 2.2.2, doping concentration plays a crucial role in determining the depletion width and minority carrier diffusion length of the betavoltaic nuclear battery, which significantly affects EHP collection efficiency and battery output performance. Figs. 6(a)-(c) illustrate the effects of N_a and N_d on J_{SC}, V_{OC}, and P_m for the proposed battery.

As shown in Fig. 6 Figure 6: see original paper, J_{SC} increases with decreasing N_a owing to its beneficial effect of expanding the minority carrier diffusion

length and depletion region width to promote EHP collection, as depicted in Fig. 3. The variation in J_{SC} with N_d is small compared with N_a because L_p is much smaller than L_n, resulting in less change in EHP collection efficiency.

Fig. 6(b) shows that V_{OC} initially increases rapidly but subsequently decreases slowly as N_a increases, as depicted in the 3D surface wireframe perpendicular to the N_d direction. The dependence of V_{OC} on N_d exhibits a similar trend. The maximum V_{OC} of 2.66 V is obtained by combining $N_a = 3.16 \times 10^{18}$ cm^{-3} and $N_d = 7.94 \times 10^{17}$ cm^{-3}. The bottom-projected contour indicates that optimal V_{OC} values are achieved at higher doping concentrations, attributed to reduction in leakage current [J_0] due to higher doping concentration, as demonstrated in Fig. S3 in Supplementary Material.

Although J_{SC} and V_{OC} exhibit opposite dependencies on doping concentration, P_m varies in the same way as J_{SC} because the variation range of V_{OC} with doping concentration is small (2.44–2.66 V with a relative increase of 8.98%). The optimal doping concentration combination is $N_a = 1 \times 10^{14}$ cm^{-3} and $N_d = 1 \times 10^{14}$ cm^{-3}, yielding the maximum output power density of 19.74 W/cm^2.

As shown in Fig. 6(d), low doping increased Q from 13.48% to 45.65% owing to widened depletion region and diffusion length, leading to longer ECR length [H_{ECR}] and improved EHP collection, resulting in higher power density. H_{ECR} and P_m follow a similar trend as Q, confirming that low doping enhances power density by increasing H_{ECR} for EHP collection. However, at the highest doping concentration, H_{ECR} and P_m are minimum, at 53 m and 6.37 W/cm^2, respectively, which are only slightly better than the power of 5.80 W/cm^2 with H_{source} of 53 m. P_m only marginally improves even with a nearly four-fold increase in source activity [A], indicating the critical role of H_{ECR} in 3D battery design and that H_{source} should not exceed H_{ECR}.

Additionally, FF ranges from 94.18% to 94.57%, with a tiny relative increase of 0.42%, while A, η_s, and $(1-r)$ remain constant at 4.04 Ci, 61.53%, and 48.77%, respectively, resulting in constant P_{in} of 129.16 W/cm^2. Therefore, Q is a significant factor affecting output power density, and low doping concentration in the P- and N-regions is recommended to enhance it, thereby maximizing short-circuit current and output power density. Detailed calculations are provided in Supplementary Material S4.

3.1.4 Critical Parameters of Device Structure

To achieve optimal device performance, we comprehensively optimized the geometric dimensions (optimization procedure #1), doping concentration (optimization procedure #2), and width of each doping layer (optimization procedure #3) of the semiconductor materials. The final optimized parameters for the battery are $N_a = N_d = 1 \times 10^{14}$ cm^{-3}, $H_P = 156$ m, $H_N = 28$ m, $t = 0.8$ m, and $d = 1.2$ m.

In optimization procedure #1, A, η_s, and $(1-r)$ exhibited significant relative increases, while relative increases in Q, V_{OC}, and FF were negligible, as shown in Fig. 7 Figure 7: see original paper. Therefore, the key factor affecting output power is the coupling of A, η_s, and $(1-r)$, and a tradeoff between them is required to maximize power density, as depicted by their optimal parameters corresponding to maximum output power.

In optimization procedure #2, A was identified as the dominant factor affecting output power, with a significant relative increase of 1204.00%, and Q was a secondary factor with a relative increase of 164.92%, as depicted in Fig. 7(b). Increasing H_P and H_N can enhance source activity [A] and ECR length. However, increasing H_P and H_N beyond the ECR leads to reduced Q, as EHPs outside the ECR become difficult to collect. The tradeoff between increasing A and decreasing Q results in saturation of output power.

In optimization procedure #3, we found that Q is the key factor affecting output power, whereas other factors have negligible relative increases, as shown in Fig. 7(c). To optimize output power density, low doping concentrations should be used in both P- and N-regions. This enables larger diffusion lengths and wider ECRs, resulting in higher EHP collection efficiency, particularly through an extended H_{ECR}.

Among these parameters, the coupling of A, η_s, and $(1-r)$ has the greatest impact on output performance, which is related to the activity, self-absorption, and backscattering of the radioactive source. The second most influential parameter is Q, which depends on the depletion region width and diffusion length controlled by doping concentration, as well as the ECR length governed by H_P, H_N, and doping concentration. To maximize output power density, use of thinner sources and converters, lower doping concentrations, and larger H_P (approximately twice the diffusion length) are recommended.

To validate the numerical model established in this study, we performed calculations on planar batteries with the same geometric dimensions and semiconductor parameters as those in references [**?**] and [**?**]; good agreement was apparent regarding output power density, as shown in Table 3 . It is worth noting that the power density of battery #1 was converted based on 100% abundance of 63Ni source, in contrast to the 20% abundance mentioned in reference [**?**]. The difference in results between reference [**?**] and this study (battery #5) is relatively large because the previous work did not consider energy loss caused by collection efficiency Q, leading to overestimation of P_m. Using our method, we can further provide suggestions for optimizing the batteries in references [**?**] and [**?**] by adjusting N_a, N_d, H_P, and H_N. For reference [**?**], setting H_P, H_N, N_a, and N_d to 4.9 m, 19.9 m, 1×10^{14} cm^{-3}, and 3.98×10^{14} cm^{-3}, respectively, the maximum output power can be increased to 296.5 nW/cm^2, representing a 12.6% improvement as depicted by battery #3. For reference [**?**], by combining $H_P = 0.1$ m, N_a and N_d at 4.7×10^{13} cm^{-3} and 3×10^{16} cm^{-3}, respectively, the output power can be increased to 378 nW/cm^2, with a 10.5% improvement as depicted by battery #6.

Finally, we conducted a comparative analysis of the P+PNN+ and PN structures, assessing their respective output power densities in 2D (#7 and #8) and 3D (#9 and #10) batteries. To achieve this, we substituted the P+ and N+ layers in the P+PNN+ structure with P and N layers of the same size to obtain the PN structure, as shown in Table 3. Our results indicate that the P+PNN+ structure outperforms the PN structure, with a 10% increase in P_m in the 2D configuration and a 39% increase in the 3D configuration. These findings highlight the superior performance of the P+PNN+ structure, particularly in 3D configurations.

In this study, diffusion lengths were calculated through commonly used equations [**?**, **?**], and the minority carrier lifetimes (τ_n and τ_p) adopted in these calculations (shown in Supplementary Material S4) fall within the range of experimental values (τ_n of 0.9–10 s and τ_p of 0.05–2.1 s) [**?**]. Moreover, experimental diffusion lengths for SiC were reported to be 30–100 m [**?**, **?**], which provides further validation for the calculated electron and hole diffusion lengths presented in this article.

3.2 Performance Simulation Using COMSOL Multiphysics

The largest discrepancies between ideal and practical performances of betavoltaic nuclear batteries are the collection efficiency Q and $V_{OC}FF/\varepsilon$ [**?**]. To better understand these discrepancies, it is necessary to conduct detailed analysis of the specific differences caused by Q, V_{OC}, and FF, as well as their underlying reasons. COMSOL Multiphysics was employed to simulate practical performance of betavoltaic batteries. Most SiC material properties were imported from the COMSOL library; properties not available in the library, such as minority carrier mobility and minority carrier lifetime, were manually added based on literature [**?**].

In the simulation process, a single converter was modeled with dimensions of 1 m × 1.2 m × 200 m. A user-controlled mesh of four different sizes (#a, #b, #c, and #d) was defined to improve both accuracy and computation time, with maximum element sizes of 50, 100, 200, and 500 nm. The minimum element sizes were set to 1/10 of the corresponding maximum element sizes. Although finer mesh sizes resulted in slightly larger P_m values, the differences are negligible. Specifically, P_m values obtained from mesh #a are only 0.064%, 0.121%, and 0.149% higher than those obtained from meshes #b, #c, and #d, respectively. Based on these results, the #d mesh was chosen for computation, with boundary elements set at maximum element size of 0.1 and minimum element size of 0.02. The maximum element growth rate was set to 1.1 with curvature factor of 0.25, and the resolution of narrow regions was specified as 1.

Fig. 8 Figure 8: see original paper displays the relationship between P_m and H_P obtained through numerical modeling and COMSOL simulations. The variations in P_m with H_P from these two methods are in excellent agreement, reaching maximum values at H_P of 156 and 164 m, respectively, with values of 19.74

and 18.69 W/cm^2, differing by only 5.62%. However, some differences in P_m at lower H_P values increase as H_P decreases. These differences arise from Q, V_{OC}, and FF, as shown in Figs. 8(a) and (b). The numerical model relies on empirical formulas (4) and (12) for Q and V_{OC}, resulting in lower Q and higher V_{OC} than the COMSOL simulation, which calculates Q by subtracting the Shockley-Read-Hall recombination rate from the EHP generation rate (shown in Fig. 8(d)) and extracts V_{OC} by finding the voltage value when current is nearly zero. In addition, the numerical model produces a higher FF with little variation, while the COMSOL simulation calculates FF by dividing P_m by V_{OC} and J_{SC}, which are sensitive to the distribution of V_{OC}.

Furthermore, P_m initially increases and then decreases with increasing H_P, reaching a maximum value at H_P of approximately $2L_n$. This can be explained by suppression of carrier recombination due to electric field distribution. The electric field distribution intensity and range at $H_P = 164$ m are much greater than those at $H_P = 4$ m, resulting in considerably lower carrier recombination rate, leading to larger Q and hence larger P_m, as shown in Fig. 8(c). This indicates that the internal mechanism affecting power increase is the electric field distribution, which governs carrier transport and collection characteristics.

The results demonstrate that the proposed battery has significantly improved output performance compared with conventional planar batteries reported in previous studies [**?**, **?**, **?**, **?**], with a maximum output power density approximately 50 times higher. If multiple batteries are stacked to a total thickness of around 10 mm, the proposed battery would provide an output power of approximately 1 mW, which can satisfy the power requirements of MEMS with dimensions less than 10 mm and power consumption of 1–100 W. We provide further recommendations for designing 3D-groove betavoltaic nuclear batteries regarding 3D etching techniques on SiC, as shown in Table S2 of the Supplementary Material.

4. Conclusions

In summary, this paper presents a novel 63Ni-SiC-based P+PNN+ 3D structure with a multi-groove design that eliminates the need for preparing a PN junction on the inner surface of the microstructure and improves the performance of betavoltaic nuclear batteries. The fully coupled model developed in this study considers various factors including β-particle generation, self-absorption, backscattering, energy deposition, radiation-induced carrier generation, and drift-diffusion, thus providing a valuable tool for efficient design and development of betavoltaic nuclear batteries with complex 3D structures. The epitaxially grown graded P/N layer significantly enhances H_{ECR}, promoting radioisotope source activity and carrier collection efficiency, producing a maximum output power density of 19.74 W/cm^2 with relatively thin radioisotope sources and converters ($t = 0.8$ m and $d = 1.2$ m), lightly doped P- and N-regions ($N_a = N_d = 10^{14}$ cm^{-3}), and longer P-region widths ($H_P = 156$ m). Analysis of carrier transport and collection characteristics using COMSOL Multiphysics provides insights into the

internal mechanism of power enhancement and clarifies discrepancies between ideal and simulated performances of betavoltaic nuclear batteries. However, diffusion length is susceptible to process variations, and a short diffusion length may reduce the advantages of the proposed P+PNN+ 3D structure. In conclusion, the proposed 3D structure with a multi-groove design, combined with a fully coupled model and optimization methods, presents a promising approach for designing and optimizing high-performance betavoltaic nuclear batteries. It is worth noting that the importance of H_{ECR} cannot be overstated in increasing output power, as it directly affects both radioisotope source loading and charge collection efficiency. Furthermore, the 3D structure proposed herein is expected to be well-suited for narrow-bandgap semiconductor materials with ultralong diffusion lengths.

See the supplementary material for details of our calculation procedure and recommendations on device design of betavoltaic nuclear batteries considering three-dimensional etching techniques on SiC.

Declaration of competing interest: The authors declare that they have no competing financial interests or personal relationships that could have influenced the work reported in this study.

Acknowledgements: This work was supported by Anhui Provincial Key R&D Program (Grant No. 202104g0102007); Jiangxi Provincial Department of Education Science and Technology Research Youth Project (GJJ200763); Hubei Provincial Natural Science Foundation of China (Grant No. 2022CFB575); Hefei Municipal Natural Science Foundation (Grant No. 2022011); Ministry of Education Industry-Education Cooperation Project (Grant No. 202102647014); Science Island Graduate Innovation and Entrepreneurship Fund Project (Grant No. KY-2022-SC-04).

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Note: Figure translations are in progress. See original paper for figures.