Maximizing output power in P-N junction betavoltaic batteries via Monte Carlo and Physics-Based Compact Model Co-Simulation

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Abstract

Betavoltaic nuclear batteries show promise as compact and enduring power sources for microelectromechanical systems (MEMS). Current theoretical calculations often overlook practical diode characteristics like surface recombination (S), bulk recombination within the space-charge region (R-SCR), series resistance (Rs) and shunt resistance (Rsh), resulting in significant gaps between theoretical predictions and experimental results, with differences in JSC, VOC, or converter efficiency up to tenfold. To address this, a Practical Diode Model, integrating these practical characteristics, is developed via Monte Carlo and Physics-Based Compact Model Co-Simulation.We quantitatively analyze the differential impacts and synergistic effects of these practical characteristics on JSC, VOC, FF, and Pout, highlighting the detrimental effects of S, R-SCR, and Rs, while emphasizing the beneficial role of Rsh. Further analysis of the degree of influence of S, Rs, and Rsh on output power reveals a priority ranking order of Rs, S, and Rsh for Si-based batteries, and S, Rsh, and Rs for SiC-based batteries. This approach effectively bridges the theoretical-experimental gap, evidenced by J-V curves closely matching tested batteries and negligible relative errors of -0.8% to 0.6% between Pout values and their tested counterparts, emphasizing its accuracy in predictions. We predict output performance across material qualities, obtaining achievable powers of 16.82 and 73.90 nW/cm2 for planar Si- and SiC-based batteries, and evaluate the quality levels of existing batteries. Furthermore, our model can forecast the performance of 3D batteries by incorporating an extended electron-hole pair generation rate model into 3D structures, achieving 28 W/cm3 for the 63Ni-Si-based multi-layer battery, surpassing planar silicon and suitable for MEMS applications.

Full Text

Preamble

Maximizing Output Power in P-N Junction Betavoltaic Batteries via Monte Carlo and Physics-Based Compact Model Co-Simulation

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Betavoltaic nuclear batteries show promise as compact and enduring power sources for microelectromechanical systems (MEMS). Current theoretical calculations often overlook practical diode characteristics like surface recombination (S), bulk recombination within the space-charge region (R-SCR), series resistance (Rs), and shunt resistance (Rsh), resulting in significant gaps between theoretical predictions and experimental results. To address this, we developed a Practical Diode Model integrating these characteristics via Monte Carlo and Physics-Based Compact Model Co-Simulation. We quantitatively analyzed the differential impacts and synergistic effects of these practical characteristics on JSC, VOC, FF, and Pout, highlighting the detrimental effects of S, R-SCR, and Rs while emphasizing the beneficial role of Rsh. Further analysis of the influence of S, Rs, and Rsh on output power reveals a priority ranking order of Rs, S, and Rsh for Si-based batteries, and S, Rsh, and Rs for SiC-based batteries. This approach effectively bridges the theoretical-experimental gap, evidenced by J-V curves closely matching tested batteries and minute relative errors of -0.8% to 0.6% between Pout values and their tested counterparts, emphasizing its accuracy in predictions. We predicted output performance across material qualities, obtaining achievable powers of 16.82 and 73.90 nW/cm^2 for planar Si- and SiC-based batteries, and evaluated the quality levels of current batteries. Furthermore, our model can forecast the performance of 3D batteries by incorporating an extended electron-hole pair generation rate model into 3D structures, achieving 28 µW/cm^3 for the 63Ni-Si-based multi-layer battery, surpassing planar silicon and suitable for MEMS applications.

Keywords: Betavoltaic nuclear battery, Physics-Based Compact Model, Monte Carlo simulation, Multi-layer structure, 63Ni, Power density

1 Introduction

The emergence of micro-electromechanical systems (MEMS) has spurred demand for micro-batteries vital for the self-sustained operation of portable or embedded micro-devices. These micro-batteries require specific characteristics: power range of 1-100 µW, sizes from 1 µm to 10 mm, and extended operational life [1]. Among these, betavoltaic nuclear batteries leveraging beta-emitting radioisotopes exhibit potential advantages including longevity, high energy density, miniature size, and robust interference resistance [2, 3].

Betavoltaic nuclear batteries function primarily through a beta radioisotope source and a semiconductor energy converter that transforms beta decay energy into electrical energy by generating electron-hole pairs, as depicted in Fig. 1 [Figure 1: see original paper]. The output power (Pout) of betavoltaic batteries is governed by source activity (A), average β-decay energy (Eavg), source efficiency (s, the ratio of β-energy emitted from the source surface to the total decay energy), and converter efficiency (c, the converter' s energy conversion efficiency), expressed as:

$$P_{out} = AE_{avg}\eta_s\eta_c$$

The converter efficiency can be expressed by $\eta_c = (1-r)QV_{OC}FFq/\varepsilon$, where r is the reflectivity coefficient, Q is the carrier collection efficiency, VOC is the open-circuit voltage, FF is the fill factor, q is the electron charge, and is the effective ionization energy to generate an electron-hole pair (EHP).

Current research focuses on selecting appropriate converters (Si, GaAs, SiC, GaN, diamond) and radioisotope sources (63Ni, 3H, and 147Pm) to maximize output power. Comparative analyses consistently demonstrate the superior performance of P-N junction betavoltaic structures over Schottky junction counterparts across various converters due to their higher built-in potential: Si-based converters showed up to 2.7 times higher efficiency [4], GaN converters displayed increased output [5], 4H-SiC converters demonstrated approximately 160% greater open circuit voltage and 50% greater power density [6, 7], and diamond converters exhibited 2.3 times greater open circuit voltage and 2.6 times greater power density [8, 9]. Beta emitters such as tritium (3H) and 63Ni are well-suited to converters, primarily due to minimum lattice damage considerations [10]. Among these, 63Ni stands out owing to its extensive half-life (approximately 100 years), moderate decay energy (Eavg = 17.4 keV, Emax = 66.9 keV), and safer handling in solid metal form.

Numerous experimental studies have investigated P-N betavoltaic batteries using converters like Si [11-14], GaAs [15, 16], SiC [6, 17, 18], and GaN [19, 20], with limited research on P-N junctions in diamonds due to challenges in n-type diamond growth techniques [8]. However, current theoretical research on P-N betavoltaic batteries often overlooks crucial practical factors inherent in battery operation, such as full energy spectrums [21], source abundance considerations [22, 23], and semiconductor material characteristics including surface states, bulk defects, and series/shunt resistance. Such oversights have resulted in significant calculation discrepancies among similar batteries and substantial gaps between theoretical predictions and experimental results.

For instance, calculated short-current density (JSC) values for Si-based converters exhibit substantial variations [24–26], ranging from 24.4 [24] to 546.8 nA/cm^2 [25] when normalized to the same source activity of 10 mCi/cm^2. Additionally, predicted c for Si, SiC, and GaN converters were anticipated to reach up to 5% [26], 23.5% [27], and 26% [28], respectively, but corresponding best experimental c was notably lower at 1.75% [29], 18.6% [1], and 2.7% [30]. Predicted VOC and FF values of 2.77 V and 94% [28] for GaN-based converters were notably higher than reported experimental values of 1.65 V and 55% [30]. Moreover, discrepancies between calculated and experimentally measured JSC and VOC values of Si-based and GaN-based converters are remarkable [14, 19, 25, 31], even reaching tenfold differences [14, 25, 31].

While preliminary explorations have examined the impact of surface recombination rates (S), bulk recombination within the space-charge region (R-SCR), and series/shunt resistance (Rs/Rsh) on battery output performance, a comprehensive and quantified systematic analysis of how these elements collectively influence batteries remains lacking. Some researchers focused solely on individual factors, such as surface recombination rates, highlighting its significant impact on parameters like Q [1] and JSC [32], but overlooked the effects of R-SCR, Rs, and Rsh. Similarly, other investigations [23, 33] utilized simulation tools like COMSOL to account for R-SCR effects but neglected crucial aspects like S, Rs, and Rsh, ultimately yielding predictions closer to ideal diodes than practical batteries. Our prior research [34] showed that elevated Rs values reduce JSC, while lower Rsh values diminish VOC and FF, yet a quantified analysis and comprehensive understanding of their underlying mechanisms remains elusive. Munson et al. [19] developed a model considering series and shunt resistance effects on GaN batteries but neglected surface recombination, leading to significant deviations from experimental values. These examples underscore the pressing need for more precise models that encompass principal practical material characteristics to narrow the gap between theoretical predictions and experimental results.

This study introduces a practical physics-based compact model, termed the Practical Diode Model, developed through Monte Carlo and Physics-Based Compact Model Co-Simulation. Utilizing Monte Carlo simulations for electron-hole pair generation rates (G(x)), this model integrates practical diode characteristics to acquire J-V characteristics for betavoltaic batteries. A comparative analysis with the Ideal Diode Model reveals differing impact mechanisms of S, R-SCR, Rs, and Rsh, allowing for quantitative analysis of their effects on JSC, VOC, FF, and Pout. We rank the importance of these factors, predict battery output performance across various material qualities (excellent, typical, and poor), and evaluate the quality levels of existing batteries. This approach effectively bridges the substantial theoretical-experimental gap, demonstrated by closely aligned J-V curves with tested batteries, emphasizing its accuracy in predictions. Furthermore, our model forecasts achievable output performance levels for 3D multi-layer betavoltaic batteries by incorporating an extended electron-hole pair generation rate model into 3D structures, providing crucial insights for designing high-performance batteries aligned with practical devices.

2.1 Device Structure and Operational Mechanism

Betavoltaic batteries convert beta decay energy into electrical energy through the drift-diffusion process of electron-hole pairs (EHPs) generated within the effective charge collection region (ECR, depicted as (Wd + Ln + Lp)) as shown in Fig. 1. The energy deposition (Edep(x)) within the converter’ s radiation transport depth [x] was calculated via Monte Carlo simulation using the Geant4 radiation transport toolkit. The process involves particle generation, source self-absorption, converter back-scattering, culminating in energy deposition within the converter. The simulation employed a rectangular 63Ni source with a full energy spectrum [24], characterized by a specific activity of 1.14 Ci/g, 20% abundance, and a density of 8.9 g/cm^3, emitting beta particles isotopically. The P-electrode adopted a grid configuration (covering about 3% of the P-surface area) to minimize energy losses of β particles, while thin passivation layers are applied to mitigate leakage current and surface recombination in other regions, as depicted in Fig. 2 Figure 2: see original paper. Figs. 2(b)-(c) illustrate the energy losses of Edep(x) within the converters attributed to electrodes and SiO$_2$ passivation layers. For a P-electrode thickness of 80 nm, the grid configuration resulted in energy losses of 0.23% and 0.21% for Si- and SiC-based converters, respectively. Meanwhile, the energy loss attributed to passivation layers increased approximately linearly with their thickness. As the passivation layer thickness increased from 10 to 200 nm, the energy losses of Edep(x) for Si- and SiC-based converters respectively rose from 0.53% to 7.86% and from 0.55% to 7.79%, with their composite losses reaching 0.53%-7.94% and 0.55%-7.88%, respectively. Consequently, our approach opted for an 80 nm thick grid configuration for the P-electrode and 10 nm thick SiO$_2$ passivation layers due to their minimal impact on Edep(x) within the converters, as seen in Figs. 2(b)-(c).

2.2 Monte Carlo and Physics-Based Compact Model Co-Simulation

The minority electron and hole concentrations n(x) and p(x) inside the PN junction diode are governed by the carrier continuity equation, which can be expressed as follows in the neutral regions of the P-type and N-type regions under steady-state:

$$\frac{\partial n(x)}{\partial t} = D_n \frac{\partial^2 n(x)}{\partial x^2} + G(x) - \frac{n(x) - n_0}{\tau_n}$$

$$\frac{\partial p(x)}{\partial t} = D_p \frac{\partial^2 p(x)}{\partial x^2} + G(x) - \frac{p(x) - p_0}{\tau_p}$$

where G(x) is the EHP generation rate, Dp (Dn) is the hole (electron) diffusion coefficient, n_0 (p_0) is the thermal equilibrium minority electron (hole) carrier concentration, and τn (τp) is the minority electron (hole) lifetime. The G(x) is determined by the energy deposition of beta particles in the converter, significantly impacting the device’ s output performance. For detailed calculations of G(x), refer to Supplementary Material S2, following our previous work methodology [23].

In the ideal diode’ s equivalent circuit (Fig. 1), part of the radiation-induced current (Jβ) flows through the PN junction diode, with the forward current (JF) equal to the diffusion current (JD), while the rest powers the load. Hence, the J-V characteristics of the ideal diode can be given by:

$$J = J_\beta - J_F$$

$$J_F = J_D = qn_i^2 \left(\frac{D_n}{N_A L_n} + \frac{D_p}{N_D L_p} \right) \left(e^{qV/kT} - 1 \right)$$

where Jβ denotes the radiation-induced current density generated by the collection of EHPs within the ECR, ni is the intrinsic carrier concentration, NA (ND) is the doping concentration in the P (N) region, Dn (Dp) is the electron (hole) diffusion coefficient, Lp (Ln) is the hole (electron) diffusion length, and J_0 is the reverse saturation current density of the ideal PN junction. The calculation methodology for Jβ has been extensively detailed in our previous studies [23]. Larger space-charge region widths (Wd) and minority diffusion lengths (Ln or Lp) promote EHP collection, thereby boosting Jβ. Lower doping concentrations have been demonstrated to increase Wd, Ln, and Lp, consequently enhancing EHP collection and Jβ. Detailed calculations of Wd, Ln, and Lp are provided in Supplementary Material S3 and S4. For detailed calculations of JD, please refer to Supplementary Material S5. In this study, we refer to Equation (3) as the Ideal Diode Model.

Significant differences [14, 25, 31] between theoretical predictions and experimental results underscore the need for a practical model that can effectively bridge this gap. Consequently, we introduce the Practical Diode Model, accounting for various practical device characteristics like surface states, bulk defects, series resistance (summing resistances in metallic contacts, surface contact resistances, and semiconductor material resistance), and shunt resistance (representing resistance from leakage and carrier-recombination, indicative of shunting loss through a conductive pathway across the P-N junction or battery edges). This model evaluates their synergistic influence on battery output performance. Our approach integrates known device characteristics, including the thicknesses and doping concentrations of individual epitaxial layers, series and shunt resistances, and the radioisotope source activity. It comprehensively considers phenomena like surface recombination and bulk recombination within the space-charge region (R-SCR), thereby enabling precise simulations that mirror real device performance. The essential input values for series and shunt resistance are obtained from J-V characterizations of practical batteries using established methodologies [35], when not explicitly available in corresponding literature.

2.2.1 Practical Diode Model for J-V Characteristics

In practical diodes, it is crucial to account for the bulk recombination current (JR) resulting from R-SCR. The net recombination in SCR can be described by the Shockley-Read-Hall statistics, then JR is mathematically defined as [36]:

$$J_R = q\int_0^{W_d} \frac{\sigma_p\sigma_n\nu_{th}N_t(n(x)p(x)-n_i^2)}{\sigma_n(n(x)+n_ie^{(E_t-E_i)/kT})+\sigma_p(p(x)+n_ie^{(E_i-E_t)/kT})}dx$$

where σn (σp) is the electron (hole) capture cross section, th is the thermal velocity, Nt is the defect density, Et is the recombination center (defect) level, and Ei is the intrinsic Fermi level. The maximum JR is given by $J_R = \frac{qn_{iW}d(e^{qV/kT}-1)}{(\tau_p+\tau_n)(e^{qV/2kT}+1)}$ when Et = Ei, where τn and τp are available in Supplementary Material S4 [2, 3].

At semiconductor device surfaces, surface defects like surface states create a space charge layer, leading to carrier recombination and establishing a concentration gradient from the bulk to the surface. This gradient generates a diffusion current, which equals the surface recombination current (JS). Consequently, the boundary conditions were given by equations (6)-(7):

$$qD_p\frac{d\Delta p(x)}{dx}\bigg|_{x=0} = qS_p\Delta p(0)$$

$$qD_n\frac{d\Delta n(x)}{dx}\bigg|_{x=W} = qS_n\Delta n(W)$$

where Sp and Sn respectively denote the surface recombination rates for holes and electrons, which are set to Sp = Sn = S in this work. By solving formulas (1) to (2) using the boundary conditions at space-charge region' s edge expressed by formulas (S10)-(S11) of the Supplementary Materials, and the front and back surfaces expressed by formulas (6)-(7) yields the expression for JS:

$$J_S = -q\frac{D_p}{L_p}(k_1 + k_{2e}^{-W_n/L_p} - \alpha L_{pk_{3e}}^{-\alpha W_n}) + q\frac{D_n}{L_n}(-m_1 + m_2 - \alpha L_{nm}3)$$

where k_1, k_2, k_3, m_1, m_2, m_3, and the detailed calculation process of JS are available in Section 6 of the Supplementary Materials.

Contrary to ideal diodes, practical diode equivalent circuits (Fig. 1) involve shunt and series resistances and the shunt resistance diverts a portion of the current (Jsh), modifying the output current to J = Jβ - JF - Jsh. Practical diodes, affected by surface recombination and R-SCR, exhibit JF = JD + JR + JS. Consequently, JF is given by:

$$J_F = J_D + J_R + J_S = J_0' \left(e^{q(V+JR_s)/nkT} - 1\right) + J_S$$

where n is the ideality factor and J_0' is the reverse saturation current density of the practical PN junction. Unlike the ideal PN junction' s reverse saturation characteristic (J_0), which considers only diffusion current at the space-charge region' s boundary, the calculation of J_0' incorporates both diffusion and recombination currents within that region. The n and J_0' are determined by fitting (JD + JR) = J_0' (exp((q(V+JR_s))/nkT) - 1), reflecting practical diode behavior where 1 < n < 2, while n = 1 in ideal diodes. Rs and Rsh are derived from J-V characterizations of practical batteries using established methods [35] when not explicitly provided in the literature. The comparison between the Practical Diode Model and Ideal Diode Model is presented in Table 1 .

JSC and VOC can be derived as V = 0 V and J = 0 A/cm^2, respectively. Subsequently, the Pout is calculated using the equation Pout = JSC VOC FF, where FF is determined based on its fundamental definition (FF = (VmJm)/(VOC JSC)). This approach of deriving FF, via the solution of d(V · J)/dV = 0 to obtain Vm and Jm, enables a more precise calculation that closely corresponds to experimental results, distinguishing it from prior approaches relying on empirical formulas. In this study, we refer to Equation (10) as the Practical Diode Model. Solving Equation (10) involves finding solutions for a complex implicit function involving multiple variables, beyond the capability of standard implicit function solvers. Hence, we employed the Newton-Raphson method to resolve it, yielding values for J and V (i.e., J-V characteristics). In the simulation process, a single converter was modeled with dimensions of 1 cm × 1 cm × 100 µm. Four mesh configurations (#a, #b, #c, #d) were tailored to balance precision and computation time, employing scaling factors ($1/10^2$, $1/10^3$, $1/10^4$, and $1/10^5$) within each iteration interval. Finer meshes offered increased accuracy but prolonged computation. The Pout values from meshes #a, #b, and #c were 1.403%, 0.138%, and 0.012% greater than that of mesh #d using the 63Ni-SiC-based betavoltaic battery reported by Zhao et al. [17]. To balance computation accuracy and time, the #c mesh was chosen for the calculation.

2.2.2 Validation of the Practical Diode Model

Accurately predicting the output performance is critical for optimizing the design of betavoltaic nuclear batteries. Hence, the validity and ability of the

Practical Diode Model to predict output performance were validated through a comparative analysis with measured results from practical batteries employing Si [11-13] and SiC [6, 17, 18] semiconductors, known as quintessential representatives of narrow-bandgap and wide-bandgap semiconductors. In the model predictions, battery parameters such as source activity and converter material or geometric parameters like doping concentration, junction depth, and junction width were set identical to the corresponding parameters of the practical devices. A summary of the relevant battery parameters can be found in Table 2 .

Figs. 3(a)-(f) confirm the reliability of the proposed Practical Diode Model, with J-V curves closely matching the original data from the tested batteries. In contrast to the significant disparities between the Ideal Diode Model and experimental values, our model effectively narrows the considerable gap between theoretical predictions and experimental results. The high R^2 values (the R-squared or coefficient of determination) of 0.995, 0.999, 0.996, 0.973, 0.937, and 0.953 for these curves demonstrate the model's accuracy in predicting the output performance of betavoltaic batteries. Table 2 further presents a meticulous comparison of all calculated Pout values against their measured counterparts with a remarkably low relative error of -0.8% to 0.6%, emphasizing the Practical Diode Model' s ability to make accurate predictions. Concurrently, it enables the estimation of essential yet unknown parameters within fabricated devices, particularly surface recombination rates (S).

3 Factors Analysis and Predictive Insights for Planar Battery Performance

3.1 Differential Impacts of Factors on Battery Performance

To unravel the determinants of battery performance, we conducted an in-depth exploration into the influence of key parameters (Rs, Rsh, S, and R-SCR) using the Practical Diode Model. Our model involved practical Si and SiC-based batteries reported by Krasnov et al. [11] and Zhao et al. [17], which are known for their exemplary output performance, with matching source activity as specified in Table 2. For Si-based betavoltaic nuclear batteries, the typical ranges of Rs, Rsh, and S were: Rs (10^4-10^6 Ω), Rsh (10^6-10^9 Ω) [11-13, 39, 40], and S (1-10^5 cm/s) [41, 42]. Detailed values for Rs and Rsh are provided in S7 of the Supplementary Materials. For SiC-based betavoltaic nuclear batteries, the ranges were: Rs (10^4-10^8 Ω), Rsh (10^6-10^{10} Ω) [17, 34], and S (10^3-10^7 cm/s) [1, 32].

Figs. 4(a)-(c) depict how Rs, Rsh, S, and R-SCR affect JSC, VOC, FF, and Pout in Si-based betavoltaic nuclear batteries. In Fig. 4 Figure 4: see original paper, JSC remains relatively constant for Rs below 10^5 Ω but significantly decreases beyond this threshold. VOC remains unaffected by Rs. The correlation of Pout with Rs follows a similar trend to that of JSC. Additionally, the recombination current density (JR) and corresponding power losses (PR) resulting from R-

SCR increase with Rs exceeding 10^5 Ω, signifying that elevated Rs increases recombination losses in SCR, resulting in substantial performance degradation.

In Fig. 4(b), JSC gradually increases and plateaus when Rsh surpasses 10^8 Ω. The dependence of VOC and Pout on Rsh mimic the pattern observed in JSC. The shunt current density (Jsh) and corresponding power losses (Psh) resulting from shunt resistance decrease with Rsh until nearly reaching zero when Rsh exceeds 10^8 Ω. Higher Rs can synergistically increase Jsh and Psh, and lower Rsh values (Rsh $< 100 \times$ Rs) or higher Rs (Rs $> 0.01 \times$ Rsh) lead to substantial performance degradation. Thus, optimal performance requires lower Rs (below 10^5 Ω) and higher Rsh (above 10^8 Ω). Fig. 4(c) reveals that JSC decreases with increasing S, with a change amplitude rising before tapering off. VOC and FF decrease with increasing S, but to a lesser extent. In contrast, JS rises with S, intensifying surface recombination and resulting in significant power losses (PS) and performance reductions. Remarkably, omitting R-SCR (w/o R-SCR) has no impact on JSC and JS but significantly increases VOC, FF, and Pout compared to considering R-SCR (w/ R-SCR), underscoring R-SCR' s substantial impact. JR mirrors JSC, resulting in notable PR and further underscoring R-SCR' s influence on Si-based betavoltaic nuclear batteries.

For SiC-based betavoltaic nuclear batteries, as shown in Figs. 4(d)-(f), the influence of Rs, Rsh, S, and R-SCR mirrors that of Si-based betavoltaic batteries. VOC increases with Rsh and saturates at Rsh = 10^9 Ω, while Pout follows a similar trend saturating at Rsh = 10^{10} Ω. In SiC-based betavoltaics, the magnitude of JR is notably smaller than that of JSC, thus power losses (PR) induced by R-SCR are significantly reduced. The shunt current density (Jsh) and corresponding power losses (Psh) decrease with Rsh until almost reaching zero when Rsh exceeds 10^{10} Ω. Optimal performance for SiC-based betavoltaics is achieved with lower Rs (below 10^6 Ω) and higher Rsh (above 10^{10} Ω). Furthermore, R-SCR has a relatively smaller impact on VOC, FF, and Pout for SiC-based betavoltaic batteries compared to Si-based batteries. Considering the synergistic effects of Rs, Rsh, S, and R-SCR reveals almost unchanged VOC and FF with S without considering series/shunt resistance (Rs = 0 Ω and Rsh = ∞), but FF exhibits a more pronounced decline when considering series/shunt resistance (Rs = 10^4 Ω and Rsh = 10^{10} Ω).

In summary, our investigation revealed that Rs significantly affects JSC and Pout, with no impact on VOC in both Si-based and SiC-based batteries. Rsh plays a substantial role in influencing JSC, VOC, Pout, and FF in both battery types. The high surface recombination rate significantly impacts JSC, VOC, Pout, and FF in both battery types. Bulk recombination within the space-charge region has a more pronounced effect on Si-based batteries compared to SiC-based batteries, highlighting the need for optimizing this aspect to mitigate its influence on battery performance. Additionally, the synergistic effects of Rs, Rsh, S, and R-SCR have a substantial impact on FF in SiC-based batteries compared with Si-based batteries.

3.2 Comparative Assessment: Practical vs. Ideal Diode Models and Influencing Factors Correlation

Table 1 compares our practical model with most reported ideal diode models on the output parameters of betavoltaic batteries. In practical diodes, the J-V curve is significantly influenced by R-SCR, often disregarded in many reported models. This influence results in a noticeable discrepancy between the forward current in practical diodes and ideal diodes, quantified through JR which grows as forward voltage increases, pushing the ideality factor n into the 1-2 range and causing J_0 to greatly exceed Ideal Diode Model predictions, as depicted in Figs. 5(a)-(b). Consequently, VOC and FF values decrease. Additionally, the impact of series and shunt resistances, as well as surface recombination, further results in a decrease in JSC and VOC, leading to significantly lower battery performance compared to values predicted by the Ideal Diode Model.

As shown in Table 2, the values of JSC, VOC, FF, and c for the Si-based betavoltaic battery predicted by the Ideal Diode Model (omitting R-SCR, series resistance, shunt resistances, and surface recombination, i.e., $JR = 0$, $Rs = 0$, $Rsh = \infty$, and $S = 0$) are approximately 1.15-2.15, 1.63-2.51, 1.23-1.44, and 3.35-4.36 times those predicted by the Practical Diode Model. In the case of SiC-based betavoltaic batteries, the values are approximately 1.07-2.24, 1.18-3.31, 1.07-1.84, and 1.82-7.07 times those obtained using the Practical Diode Model. These observations highlight the precision of our model in calculating VOC and FF by incorporating these practical material characteristics, aligning closely with experimental results.

Furthermore, analyzing the impact of Rs, Rsh, and S on battery performance via the Practical Diode Model, we observe distinct trends based on the results from the heat map analysis depicted in Figs. 5(c)-(d). Rs shows a positive correlation with JR and Jsh while exhibiting a negative correlation with JSC, FF, and Pout. This indicates that an increase in Rs enhances R-SCR and shunt loss, leading to a decrease in battery performance. Rsh demonstrates a weaker positive correlation with JSC, VOC, FF, and Pout for Si-based batteries, but it displays a strong positive correlation with VOC, FF, and Pout for SiC-based batteries, indicating a higher sensitivity of SiC-based batteries to Rsh compared to Si-based ones. The increase in Rsh reduces shunt loss, leading to an improvement in battery performance. S exhibits a strong negative correlation with JSC, Jsh, VOC, and Pout, highlighting the significant impact of surface recombination rate on battery performance and indicating a competitive mechanism between surface recombination and shunt resistance. Specifically, S shows a strong negative correlation with JR, and JR exhibits a robust negative correlation with Pout for Si-based batteries, further confirming that R-SCR in Si-based batteries is stronger than that in SiC-based batteries.

In summary, for Si-based batteries, the impact on output power ranks in the order of Rs, S, and Rsh. However, for SiC-based batteries, the impact on output power follows the order of S, Rsh, and Rs. The synergistic effects of Rs, Rsh, and

R-SCR contribute to the gap between theoretical predictions and experimental results in betavoltaic batteries.

3.3 Predicting Output Performance across Various Material Qualities and Evaluating Current Battery Qualities

Our Practical Diode Model effectively validates the influence of practical material characteristics (S, R-SCR, Rs, and Rsh) and their impact on battery output performance. By considering these characteristics, we bridge the substantial gap between theoretically calculated performance and experimental results. This approach also sheds light on the current state of battery manufacturing processes. Based on typical ranges of Rs, Rsh, and S reported by previous studies [1, 12, 17, 32, 34, 39, 41, 42], we categorized practical material characteristics into three levels: low, medium, and high, as shown in Table 3 . Given that series resistance is usually lower than shunt resistance [43], we divided practical material quality into three levels: Excellent (Rs = 10^5 Ω, Rsh = 10^8 Ω, and S = 10 cm/s for Si-based batteries; Rs = 10^4 Ω, Rsh = 10^{10} Ω, and S = 10^3 cm/s for SiC-based batteries), Typical (Rs = 10^6 Ω, Rsh = 10^7 Ω, and S = 10^3 cm/s for Si-based batteries; Rs = 10^6 Ω, Rsh = 10^9 Ω, and S = 10^5 cm/s for SiC-based batteries), and Poor (Rs = 10^6 Ω, Rsh = 10^6 Ω, and S = 10^5 cm/s for Si-based batteries; Rs = 10^8 Ω, Rsh = 10^8 Ω, and S = 10^7 cm/s for SiC-based batteries).

Our Practical Diode Model underwent optimization across various material characteristics. Omitting considerations for R-SCR, S, Rs, and Rsh (i.e., ideal diodes) resulted in Pout values of 25.30 nW/cm^2 and 113.11 nW/cm^2 for Si- and SiC-based batteries, respectively. Corresponding c were 6% for Si-based batteries and 27.16% for SiC-based batteries. When considering only R-SCR but neglecting S, Rs, and Rsh (i.e., limit quality), the Pout of Si- and SiC-based batteries remained at 17.98 nW/cm^2 and 96.25 nW/cm^2, respectively. Their corresponding c were 4.27% for Si-based batteries and 23.11% for SiC-based batteries, respectively.

Encompassing R-SCR, S, Rs, and Rsh led to variable outcomes in Pout and c across different material qualities. For Si-based batteries, this resulted in 16.82 nW/cm^2 and 3.99% (excellent quality), 9.31 nW/cm^2 and 2.21% (typical quality), and 0.89 nW/cm^2 and 0.21% (poor quality). In contrast, for SiC-based batteries, the values stood at 73.90 nW/cm^2 and 17.74% (excellent quality), 23.54 nW/cm^2 and 5.65% (typical quality), and 2.78 nW/cm^2 and 0.67% (poor quality). The substantial performance disparity between practical diodes across different qualities and ideal diodes highlights the consequence of neglecting practical material characteristics, leading to an overestimation of Pout and c. Additionally, the optimal output performance of batteries with various material characteristics is achieved at different doping concentrations, providing valuable insights for guiding the optimization of battery fabrication processes.

In current technological capabilities, Si and SiC batteries can achieve respective output powers of 16.82 nW/cm^2 and 73.90 nW/cm^2, with c reaching 3.99% and 17.74%. Additionally, c increases as the source thickness decreases, nearing the material’ s limiting efficiency. Assessing battery quality based on c, batteries reported by prior investigations can be evaluated accordingly, as shown in Fig. 6 [Figure 6: see original paper]. The quality of SiC-based battery reported by Zhao et al. [17] closely approximates excellent quality, albeit with slightly higher Rs values. The quality of Si- [11] and SiC-based [6, 18] batteries examined in prior investigations closely approximates typical quality, primarily influenced by increased Rs, diminished Rsh, or elevated S. Notably, the Si-based batteries examined in studies [12, 13] tend towards poorer quality, primarily due to significantly higher S. This highlights the critical need for optimizing battery performance by refining processes targeting reduced resistance, surface recombination rates, and shunting loss through conductive pathways.

4 Predicting and Optimizing Output Performance for Multi-layer Structure

Conventional planar betavoltaic batteries face limitations due to one-sided isotope source usage and strong self-absorption effects, restricting their output power to the nW range (Table S1 in Supplementary Material). In contrast, 3D structures hold the promise of high-power generation through increased specific surface area and conversion efficiency [37, 44–46]. Accurate theoretical predictions for battery output performance play a crucial role in guiding the preparation and optimization processes for 3D betavoltaic batteries. Despite differences in the spatial distribution of the EHP generation rate (G(x)) within converters, the operational principles of 3D batteries align with those of planar batteries, following the same carrier continuity equation and physical laws. By extending G(x) from 2D to 3D structures, our Practical Diode Model can be adapted for predicting the output performance of 3D batteries.

We introduce a multi-layer design to substantially enhance battery output performance by increasing A s(1 - r). This design utilizes 3D stacked multi-layer structures, leveraging both sides of the isotope source, increasing cells per unit thickness, and enhancing source surface activity. Leveraging our Practical Diode Model and considering practical material characteristics, we optimize this multi-layer structure for enhanced performance.

4.1 Multi-layer Structure and Modeling EHP Generation Rates

The proposed structure for a 63Ni-based betavoltaic battery with multi-layers characterized by a converter-source-converter sandwich structure is illustrated in Fig. 7 Figure 7: see original paper. A dual-emitting self-supporting 63Ni sheet is sandwiched between two symmetric converters with P-N junction to form a sandwich basic unit (SBU). Uj denotes the j-th SBU, Sj indicates the j-th 63Ni sheet, and Dj,1 (Dj,2) denotes the upper (lower) converter of the j-th SBU. Within a 1 cm × 1 cm rectangular area, the thickness of the 63Ni sheet and converter in each layer are denoted as t and d, respectively. We chose silicon as the converter material due to its advanced thinning technology, reduced to 4 µm [47], compared to 30 µm for SiC [48]. For effective battery operation, the interconnection of SBUs is crucial, requiring the establishment of Ohmic contacts on converters. Based on Figs. 2(b)-(c), we adopted 80 nm grid-shaped electrodes for both the P- and N-regions, along with 10 nm SiO_2 passivation layers due to their minimal impact on the energy losses within the converters. The composite energy losses induced by electrodes and passivation layers ranged from 0.56% to 1.2% as the passivation layer thickness increased from 10 to 20 nm. Further details on calculating composite energy losses and employing electrode and passivation layers are provided in S8 of the Supplementary Materials.

To accurately model the energy deposition and EHP generation rate in a multilayer betavoltaic nuclear battery, it is essential to consider the superposition contributions of all the isotope sources, converters, and passivation layers. This involves extending G(x) of the 2D structure to that of the 3D structure (i.e., G(x, t, d, H)). Fig. 7(b) characterizes the penetration distance distribution of β particles released by 63Ni isotope sources. At a random location of the EHPs generated in converter Dj,1 (specified by reference site P), the distance between P and source Sj is represented by [x]. Dj,1 is irradiated by the upper (j - 1) isotope sources, and the β particles emitted from the i-th (i < j) source need to penetrate a total source thickness of (j - i - 1)t, a total converter thickness of [2(j - i)d - x] and a total passivation-layer thickness of [(4(j - i) - 1)H] to reach the reference site P. Similarly, Dj,1 is irradiated by the lower (m + 1 - j) layers of sources, and the β particles emitted from the k-th (j ≤ k ≤ m) source need to penetrate a total source thickness of (k - j)t, a total converter thickness of [2(k - j)d + x] and a total passivation-layer thickness of [(4(k - j) + 1)H] to reach the reference site P. During this process, the energy of beta particles decays exponentially with penetration distance; hence Gj,1(x, t) can be expressed by:

$$G_{j,1}(x,t,d,H) = \sum_{i=1}^{j-1} G_0(t) e^{-\alpha(t)(2(j-i)d-x)} e^{-\gamma_1(t)(j-i-1)t} e^{-\gamma_2(t)(4(j-i)-1)H} + \sum_{k=j}^{m} G_0(t) e^{-\alpha(t)(2(k-j)d+x)} e^{-\gamma_1(t)(k-j)t} e^{-}$$

where m is the number of SBUs, $G_0(t)$ is the surface electron-hole pair generation rate, $\alpha(t)$ is the absorption coefficient of β-electron flux in Si, $\gamma_1(t)$ is the absorption coefficient of β-electron flux in 63Ni and $\gamma_2(t)$ is the absorption coefficient of β-electron flux in passivation-layer, which are acquired via the equation in Table 5 based on Monte Carlo code simulation. The electron-hole pair generation rate of converter Dj,2 can be expressed as G(j,2)(x, t, d, H) = G(n+1-j,1)(x, t, d, H) due to the symmetries of the multi-layer structure. Table 5 illustrates R^2 (R-squared or coefficient of determination) values exceeding 0.99, signifying excellent model fitting.

Accurate prediction of EHP generation rates is crucial for optimizing 3D multilayer betavoltaic batteries. Validating our model, represented by formula (11), against original Geant4 data, Figs. 8(a)-(c) reveal the model' s reliability. The R^2 values (0.983, 0.981, and 0.971) for different t and d affirm its accuracy in estimating EHP generation rates within 3D multi-layer structures, which establishes its significance as a key tool for developing high-performance betavoltaic batteries. While it is worth noting that the fitted values at the converter' s surface are lower than the actual values, this discrepancy has a minimal impact on the overall energy distribution in converters.

4.2 Optimization of Multi-layer Structure for Enhanced Performance

To optimize the structure of the proposed battery and maximize its output power density, a parametric sweep was conducted in the practical physics-based compact model to adjust variables including the single-source thickness (t) and single-converter thickness (d), acceptor concentration of P-region (NA), and donor concentration of N-region (ND). The feasible doping concentration NA and ND can range from 1×10^{14} to 1×10^{20} cm^{-3} and 1×10^{14} to 1×10^{19} cm^{-3}. Possible thicknesses (t and d) are defined as 0.1–5 μm and 0.5–10 μm, respectively, with a 0.01 μm step size for each, according to the 63Ni source self-absorption and the energy deposition depth of beta particles in the converter, as shown in Figs. S1(a) and (b) of the Supplementary Material. We select a junction depth of 0.3 μm due to our facility' s capacity to process shallow junctions. To investigate the impact of the number of SBUs on output performance, we assess the multi-layer battery' s power using volume power density.

4.2.1 Optimization of Source and Converter Thicknesses The output power can be defined as the converter efficiency multiplied by the power absorbed in the device (input power, Pin) [49]. Therefore, the battery output performance can be evaluated by input power due to the converter limiting efficiency of the same material being a constant [38]. To find the optimal geometric structure parameters for the battery, we maximize Pin by optimizing t and d using equation (12):

$$P_{in}(t,d,n) = \frac{A \cdot \int_0^{W_d} E_{dep}(x,t)dx}{V} = \frac{m(t+2d+4H')}{SA}$$

where Edep is the energy absorbed in the converters, V is the volume of the stacked multi-layer battery, H' is P-(N-) electrode thickness which was set as 80 nm, and SA is the junction area (1 cm^2).

Fig. 9 Figure 9: see original paper illustrates the relationship between the maximum Pin and m. It's evident that Pin increases significantly with increasing m until it saturates at m = 25. A larger m corresponds to a greater number of sources within the beta particle range in the battery. This results in more decay energy being deposited in a specific converter until the distance between this converter and the added sources exceeds the beta particle range. For subsequent calculations, the number of SBUs is set to 25.

The 3D surface wireframe depicted perpendicular to the d direction in Fig. 9(b) reveals that Pin initially rises swiftly but subsequently decreases as t increases, reaching a peak value at t = 0.6-2.8 µm. Similarly, the relationship of Pin with d shows a similar trend, peaking at d = 0.6-2.2 µm. The bottom projected contour demonstrates that the optimal Pin values are achieved within the range of 0.4-2 µm for d and 0.5-1.8 µm for t. The maximum Pin of 845.73 $\mu W/cm^3$ is obtained at t = 1.1 µm and d = 1.1 µm. However, considering the current Si thinning technology level (d = 4 µm) [47], the maximum Pin of 583.09 $\mu W/cm^3$ is reached at t = 2.2 µm.

Fig. 9(c) demonstrates the spatial distribution of Pin in converter Dj,1 (the upper layer of the j-th SBU) and Dj,2 (the lower layer of the j-th SBU), with j ranging from 1 to 25. Pin is lowest in converter D1,1, the outermost layer, and progressively increases as the converter goes deeper until it saturates. Pin tends to saturate at the converter D2,2 for t = 1.1 µm and d = 1.1 µm, whereas it tends to saturate at the converter D1,2 for t = 2.2 µm and d = 4 µm. This discrepancy could be attributed to the limited contribution of sources far from a specific converter when both the source and converter are sufficiently thick.

The input power can be computed by integrating A, s, and r as Pin = A ·Eavg · s ·(1 - r). Fig. 9(d) depicts the impact of varying source thicknesses (t) on A, s, r, and A s(1 - r). With increasing t, s decreases from 0.92 to 0.16, while r shows slight variation (0.22 to 0.29). A exhibits a linear increase with t. The trends in Pin and A s(1 - r) with respect to t align, emphasizing Pin is determined by the coupling of A, s and r. In our proposed battery design, higher t values enhance A but reduce s due to self-absorption. Striking a balance between A, r, and s is pivotal for optimizing power density.

4.2.2 Optimization of Doping Concentration in P-N Junction We examined the impact of doping concentration (ND and NA) on JSC, VOC, and Pout across various quality levels: poor, typical, and excellent, comparing their performance to ideal diodes.

In Fig. 10 Figure 10: see original paper, for the battery with ideal diodes (ideal quality), at a certain NA, JSC remains relatively stable with increasing ND at lower doping levels within the N-region, and subsequently decreases with higher ND. Similarly, JSC exhibits analogous trends with NA at a specific ND. VOC increases with ND but diminishes at higher ND doping levels. Pout follows the same trend as VOC, peaking at NA = 2.51×10^{19} cm^{-3} and ND = 7.94×10^{17} cm^{-3}, reaching 44.2 $\mu W/cm^3$. Since Ln is longer than Lp when the doping concentration exceeds 10^{19} cm^{-3}, as depicted in Fig. S3 of the supplementary materials, NA greater than ND is more conducive to carrier collection, boosting output power density.

In Fig. 10(b), for excellent quality batteries, JSC initially rises gradually with

ND but later declines. VOC and Pout initially rise with ND within the NA range of 10^{16}-10^{20} cm^{-3}, then exhibiting a swifter decline, reaching their peaks at lower ND. Conversely, at lower NA, VOC and Pout exhibit slower changes, reaching their maxima at higher ND. Overall, Pout peaks at 28.22 μW/cm^{3} at NA = 1.58×10^{18} cm^{-3} and ND = 7.94×10^{14} cm^{-3}.

For typical quality batteries (Fig. 10(c)), at a specific NA, JSC initially rises gradually with ND, followed by a decline. While, at a specific ND, JSC increases with NA. The relationships between VOC and Pout with respect to ND mirror those observed in excellent quality batteries, reaching a maximum Pout of 14.23 μW/cm^{3} at NA = 2.51×10^{19} cm^{-3} and ND = 7.94×10^{14} cm^{-3}.

In Fig. 10(d), for poor-quality batteries, JSC, VOC, and Pout exhibit minimal variation at lower ND doping levels, subsequently decreasing with increasing ND, achieving a maximum Pout of 1.22 μW/cm^{3} at NA = 1×10^{20} cm^{-3} and ND = 1×10^{14} cm^{-3}.

Overall, battery performance across quality levels exhibits distinct correlations with doping concentration. Ideal diodes show optimal performance at higher doping levels in both P- and N-regions, while practical batteries exhibit their best performance at higher P-region and lower N-region doping levels. Ideal diodes yield a Pout of 44.2 μW/cm^{3}, disregarding practical material characteristics. However, considering these characteristics, VOC and FF decrease significantly, leading to substantial reductions in Pout (Table 6). Compared to ideal batteries, Pout drops by 56.6%, 210.7%, and 3508.7% for excellent, typical, and poor-quality batteries, respectively. Similarly, the overall conversion efficiency (tot, tot = s c) and c also exhibit the same reduction rates, highlighting the overestimation of ideal diodes.

Comparing the output performance of the multi-layer silicon (PN) battery utilizing our Practical Diode Model with the predictions from previous research [37] under the same structural parameters and source activity (100% abundance of 63Ni source), we observed that when excluding considerations for RSCR, S, Rs, and Rsh (i.e., ideal diodes), our obtained Pout of 435 μW/cm^{3} closely aligns with the previous research' s prediction of 437 μW/cm^{3}. When considering only RSCR but not S, Rs, and Rsh (i.e., limit quality), the Pout is 193 μW/cm^{3}. However, when considering RSCR, S, Rs, and Rsh, the Pout varies with different material qualities—187 μW/cm^{3} (excellent quality), 135 μW/cm^{3} (typical quality), and 17 μW/cm^{3} (poor quality). This notable disparity is attributed to the omission of practical material characteristics, leading to an overestimation of JSC, VOC, and FF. Our Practical Diode Model holds the potential to bridge the gap between theoretical predictions and experimental results, offering an accurate method for designing high-output power batteries. Moreover, our multi-layer silicon (PN) battery design, based on the converter-source-converter sandwich basic unit, facilitates parallel or series connection as well as assembly.

In summary, our Practical Diode Model optimized the multi-layer battery across various material characteristic levels. Leveraging high-level semiconductor fabrication (excellent quality) and radioisotope source preparation technology, the multi-layer battery achieved a Pout of approximately 28.22 µW/cm^3, significantly surpassing the 0.94 µW/cm^3 of corresponding conventional planar silicon (PIN) batteries (as indicated in Table 6). With further stacking, Pout could meet MEMS power requirements. With a 100% abundance of the 63Ni source, Pout could reach around 162 µW/cm^3.

5 Conclusions

Our study presents a comprehensive framework for evaluating and optimizing betavoltaic battery performance. The implementation of the Practical Diode Model incorporates critical factors: practical sources characteristics (full energy spectrum, abundance, self-absorption, back-scattering), diode characteristics (surface recombination, bulk recombination, series resistance, shunt resistance), and energy losses related to electrodes and passivation layers. This integration effectively bridges the gap between theoretical projections and experimental outcomes, offering a precise tool for battery design.

Analysis reveals that Rs and S significantly impact battery performance negatively, with Rs exacerbating surface recombination. Conversely, Rsh demonstrates a relatively positive effect. Notably, bulk recombination more acutely affects Si-based batteries compared to SiC-based ones. The prioritization of these factors reveals an order of Rs, S, and Rsh for Si-based batteries, while in SiC-based batteries, Rsh and S outweigh the impact of Rs. Evaluation of current batteries indicates varying quality levels, attributing poorer quality to high Rs and S. Predictions of battery output performance across various material qualities and within existing technological capabilities indicate that Si- and SiC-based batteries can achieve respective output powers of 16.82 and 73.90 nW/cm^2, with c reaching 3.99% and 17.74%. Further optimization of Si-based multi-layer structures, leveraging high-level semiconductor fabrication (excellent quality), yielded significant improvements in battery output-power (28 µW) suitable for MEMS applications. Our study elucidates critical connections between practical material characteristics, source and converter parameters, and battery performance. This work establishes a robust framework aligning theoretical predictions with experimental outcomes in betavoltaic battery evaluation and optimization.

Author Contributions

Houjun He: Conceptualization (equal); Formal analysis (lead); Investigation (lead); Methodology (lead); Software (lead); Visualization (lead); Writing –original draft (lead); Writing –review & editing (equal).
Yuncheng Han: Conceptualization (equal); Funding acquisition (lead); Supervision (equal); Writing –review & editing (equal).
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Lei Ren: Writing –review & editing (equal).

Xiangdong Meng: Writing –review & editing (equal).
Mingjie Zheng: Conceptualization (equal); Supervision (equal).

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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