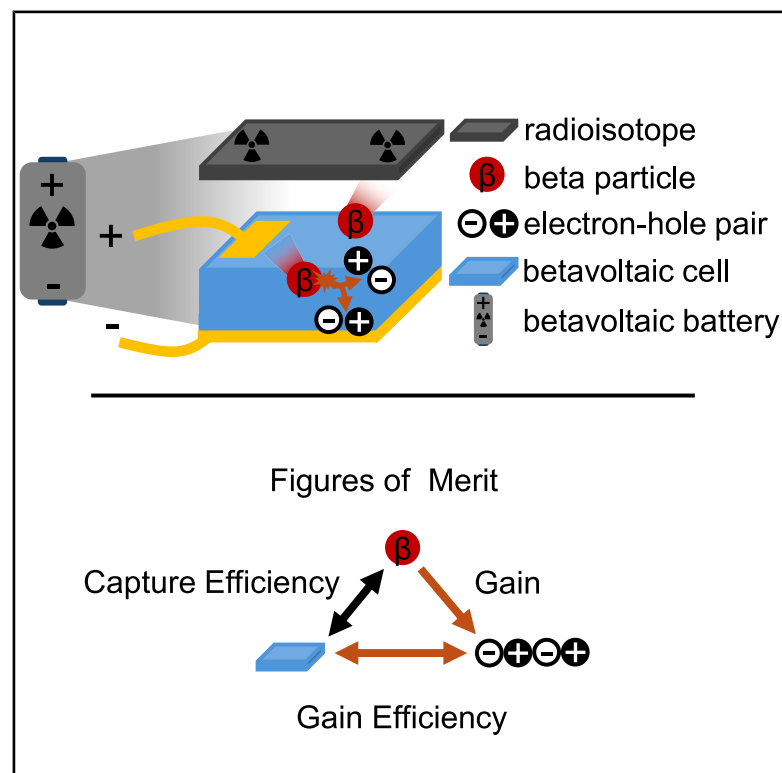


Figures of merit to quantify betavoltaic device performance

Graphical abstract



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In brief

Betavoltaic energy conversion uses semiconductors to convert beta radiation from radioisotopes into electricity. Many combinations of semiconductors and radioisotopes can be used, resulting in variations in conversion efficiency among technologies. We introduce energy-resolved figures of merit to standardize characterization. These metrics are technology independent, enabling cross-platform comparisons.

Highlights

- Energy-resolved figures of merit for betavoltaic cells are introduced
- Capture efficiency measures power transmission efficiency as a function of energy
- Gain quantifies the current multiplier effect as a function of energy
- Gain efficiency measures carrier collection as a function of energy



Article

Figures of merit to quantify betavoltaic device performance

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SUMMARY

Betavoltaic energy conversion is a specialized energy harvesting technology using a semiconductor to convert beta radiation from a radiation source into continuous electricity. Many semiconductor materials and radioactive isotopes are viable, making it challenging to benchmark technologies. To facilitate comparison, modeling, and characterization, we introduce three figures of merit: capture efficiency, gain, and gain efficiency. We showcase these metrics by numerically modeling the performance of GaAs, SiC, and GaN p-n and p-i-n junctions under ³H and ⁶³Ni radioisotope irradiation. The capture efficiency describes the energy fraction that can be absorbed by the cell. The gain and gain efficiency quantify carrier multiplier effects and carrier collection effectiveness. The figures of merit study indicates that (1) absorber materials with low atomic numbers improve energy capture in the cell and (2) single-junction betavoltaics do not require complete radiation absorption to obtain maximum operating efficiency.

INTRODUCTION

Betavoltaics is an energy harvesting technology that generates electricity by converting beta emissions into an electric current. Betavoltaic devices are comprised of a beta radiation source and a semiconductor, as illustrated in Figure 1A. This process produces electron-hole pairs inside the semiconductor, similar to a photovoltaic cell when illuminated with light. These devices can have very long lifetimes, depending on the half-life of the radioisotope used as the beta radiation source. A long operational life is relevant to applications where battery recharging is challenging, such as intracutaneous¹ (Figure 1B), deep sea (Figure 1C), and outer space environments.

Commonly used radioactive isotopes in betavoltaics include tritium (³H)^{2–6} and ⁶³Ni.^{3,4,7–14} To avoid problems with leakage of tritium gas, it is preferred to store tritium as a metal tritide.^{15,16} Multiple semiconductors have been investigated for betavoltaics, including GaAs,^{3,4,7,9,17–20} SiC,^{2,14,17,18,21–24} and GaN.^{3,8,17–20,25,26} Betavoltaic technology is limited to a theoretical conversion efficiency ranging between 5% and 30%, depending on the semiconductor used.^{3,19,27} Loss mechanisms in betavoltaics have been studied previously, and multiple figures of merit have been proposed, such as the coupling efficiency and the semiconductor conversion efficiency, to quantify performance.^{3,17,19,27} Betavoltaic cells, like photovoltaic cells, can also be characterized with performance metrics such as the open circuit voltage (V_{oc}), the short circuit current density (J_{sc}), and the maximum power density (P_{max}). These figures of

merit provide rich information on each specific radioisotope-semiconductor combination and the cell performance. However, since established metrics describe the performance of a device operating under the full radioisotope spectrum, they are inadequate to characterize properties that depend on the beta particle energy. Different absorber materials and radioisotopes lead to significant differences in performance, making direct comparisons across technologies challenging. Different isotopes emit beta particles across distinct energy spectra, and these particles interact with absorbers in ways that depend on both their energy and the properties of the absorbing material. To ensure fair comparison, beta particle energy-resolved figures of merit are required.

In this work, we propose three energy-dependent figures of merit to assess betavoltaic cell performance: the capture efficiency, the gain, and the gain efficiency. The capture efficiency describes the energy fraction that can be absorbed by the cell as a function of beta particle energy. The gain is the carrier generation amplification relative to incident particle flux, defined as the ratio between J_{sc} to absorbed beta particle flux. The gain efficiency quantifies carrier collection effectiveness as a function of beta particle energy. Figure 1D presents the relationship between the three figures of merit. These performance parameters facilitate comparison between technologies, device optimization, and characterization. To demonstrate how these metrics can elucidate power losses in betavoltaic devices, we model GaAs, SiC, and GaN p-n and p-i-n betavoltaic cells under ³H and ⁶³Ni irradiation. The model includes Monte Carlo simulations



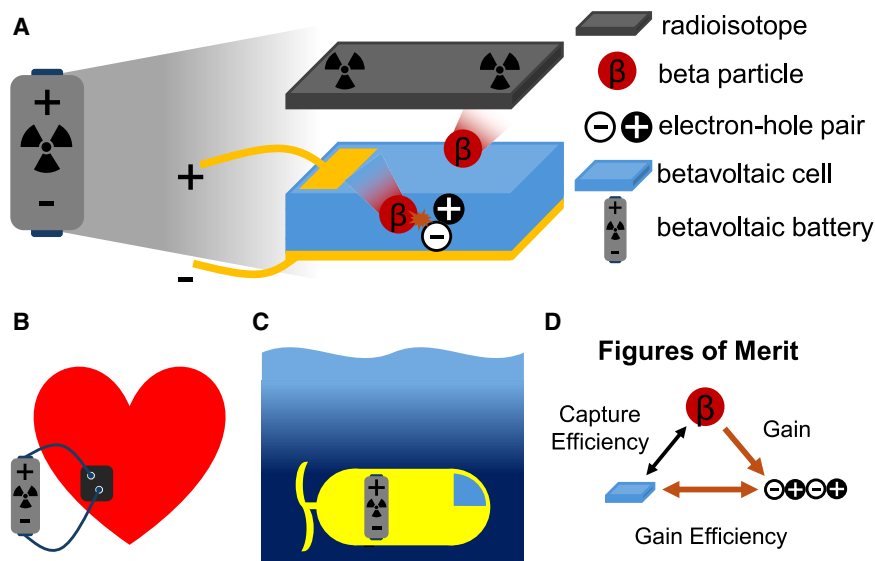


Figure 1. Betavoltaic battery and its applications

(A) Schematic of the constituents of a betavoltaic battery.

(B and C) Applications of betavoltaic batteries include (B) pacemakers and (C) deep-sea applications.

(D) Visual relationship between the three figures of merit. The black arrow describes the interactions between the radioisotope and the betavoltaic cell, and the orange arrows describe the interactions within the betavoltaic cell.

to assess the electron-matter interactions between beta particles and semiconductor heterostructures. Drift-diffusion calculations evaluate the carrier collection and device performance. The model is validated against experimental results (see details under [methods](#)). A particle swarm algorithm finds the optimal layer thicknesses and semiconductor doping levels for the p-n and p-i-n structures under both radioisotopes.

RESULTS

Impact of the radioisotope spectrum on electron-hole generation rates

The hydrogen radioisotope tritium (^3H) and the nickel radioisotope (^{63}Ni) have different beta particle emission spectra. The spectra are shown in [Figure 2A](#) for ^3H and [Figure 2B](#) for ^{63}Ni . ^3H can emit beta particles between 0 and 18 keV, whereas ^{63}Ni emits, on average, beta particles that are more energetic, reaching 66 keV. When they arrive in a semiconductor, each particle creates a cascade of secondary electrons that can contribute toward the generated current. After the secondary electrons are produced, a p-n or p-i-n structure is used to collect the carriers. The thickness of the layers must be chosen carefully, with a thick junction allowing absorption of all beta particles and a thin junction increasing the collection of generated carriers. [Figures 2C](#) and [2D](#) illustrate the electron-hole pair generation rate in a GaAs betavoltaic cell created under ^3H and ^{63}Ni , respectively, as a function of the depth into the cell. The carrier generation profiles were obtained by combining Monte Carlo simulations of beta particle emission and a radiation ionization conversion software, following the empirical relationship established by Klein,²⁸ as described under [methods](#). Under ^3H , most of the carriers are generated within the first 2 μm of the surface. Since ^{63}Ni emits, on average, more energetic beta particles, carriers are generated beyond 10 μm . Schematics of optimal p-n heterostructures are shown in [Figures 2C](#) and [2D](#), matching the depth on the horizontal axis.

are generated within the junction. The remaining carriers are generated deeper in the device and do not contribute toward the device current. The generated carriers are limited by a diffusion length of $\approx 2.2 \mu\text{m}$ in the optimal device for ^{63}Ni , meaning that even if they are absorbed, they may not be collected. In other words, due to the large beta particle penetration depths, bulk recombination can hinder device performance. This finding suggests that the tradeoff between thick junctions for maximal radiation absorption versus thin junctions to limit bulk recombination is different depending on the radioisotope.

Betavoltaic and photovoltaic performance are both affected by limiting physical phenomena, such as electron-hole pair recombination. In photovoltaics, a well-known tradeoff is that the thicker the absorber layer, the larger the number of photons absorbed, but it limits carrier collection, as they have to travel farther before finding the junction. The same tradeoff occurs in betavoltaics, where carriers can only be collected if the beta particles are stopped in the p and n absorber layers. Increasing the thickness of those layers increases carrier generation but decreases carrier collection, just as in photovoltaics. We show that the optimal absorber thickness depends significantly on the beta particle energies produced by the radioactive source. The active-layer thicknesses and doping levels must therefore be tailored to the nature of the isotope to maximize conversion efficiency. For this purpose, we define figures of merit that aid in understanding optimal betavoltaic absorber thicknesses.

Capture efficiency in betavoltaic cells

The capture efficiency describes the energy fraction that can be absorbed by the betavoltaic cell as a function of beta particle energy (see details under [methods](#)). [Figure 2E](#) depicts the capture efficiency for SiC, GaN, and GaAs as absorber materials as a function of beta particle energy. Energy loss mechanisms limiting the capture efficiency can be attributed to backscattering, secondary electrons escaping the cell, and photon emission. The energy dependence of the capture efficiency reveals

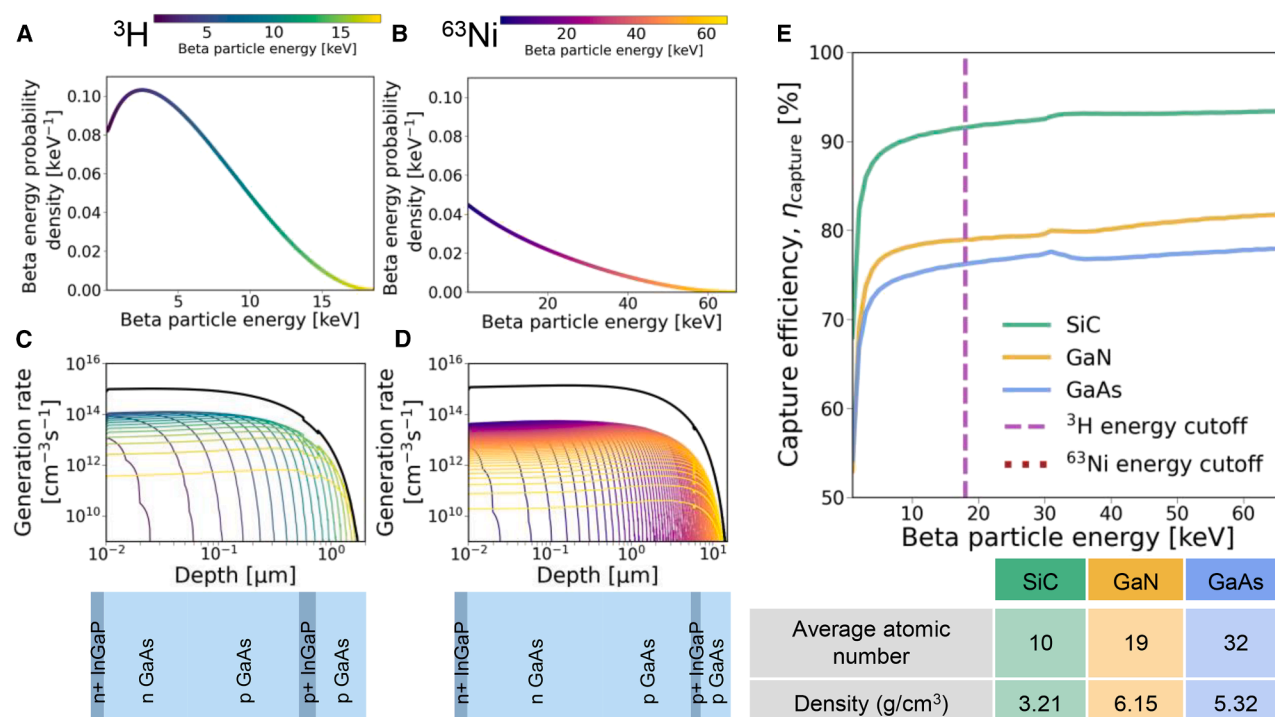


Figure 2. Radioisotope emission probability spectrum, capture efficiency, and electron-hole pair generation rates

(A and B) Radioisotope emission probability spectrum for (A) ^3H and (B) ^{63}Ni .

(C and D) The electron-hole pair generation rate as a function of the depth into the heterostructure for ^3H and ^{63}Ni . Each color represents the generation rate created by beta particles summed within a 1 keV window, matching the color bar at the top. The black line corresponds to the total generation rate summed over the full radioisotope spectrum.

(E) The capture efficiency of the energy in the betavoltaic device as a function of beta particle energy. The beta particle energy for ^3H reaches 18 keV, as indicated by the purple vertical dashed line, and it reaches 66 keV for ^{63}Ni , as indicated by the dark red vertical dashed line.

that losses occur at lower beta particle energy. This phenomenon is explained by a larger number of secondary electrons escaping the cell at low energy.²⁹ Furthermore, the electron mean free path increases with energy, meaning that the backscattering coefficient is expected to be higher at low beta particle energy (1–10 keV).³⁰

These mechanisms have an impact on the radioisotope choice. For example, ^{63}Ni enables capture efficiencies 3%–4% higher on average than ^3H , depending on the cell material. ^3H has a lower average capture efficiency than ^{63}Ni because the reduction at low beta particle energy (1–10 keV) is more significant on the narrow (up to 18 keV) ^3H spectrum than it is on the large (up to 66 keV) ^{63}Ni spectrum. This behavior is consistent with coupling efficiencies reported previously.³

The capture efficiency can also identify promising absorber materials. The capture efficiency is larger for SiC than GaN or GaAs due to the lower effective atomic number and material density, as indicated in Figure 2E. This behavior is consistent with previous studies reporting that the backscattering coefficients increase with atomic number.³¹ Therefore, using semiconductors with low effective atomic numbers and low densities can improve capture efficiency. This suggests that engineering metamaterials to artificially reduce the density could increase the capture efficiency. This figure of merit enables benchmarking these future improvements. However, engineering material

properties may adversely affect other key performance indicators, such as gain and gain efficiency. Therefore, a careful optimization process that balances all relevant figures of merit is essential. GaAs is chosen as the absorber material for the subsequent gain and gain efficiency analysis, as it is an established benchmarking technology for energy conversion systems such as photovoltaics.

Gain and gain efficiency in betavoltaic cells

The gain is the carrier generation amplification relative to incident particle flux, defined as the ratio between J_{sc} to absorbed beta particle flux. The gain efficiency quantifies carrier collection effectiveness as a function of beta particle energy. The detailed calculations can be found under methods. Figure 3 presents the gain of the optimized p-n and p-i-n GaAs betavoltaic cells under ^3H (Figure 3A) and ^{63}Ni (Figure 3B) compared to Klein's limit. The gain efficiency is illustrated in Figures 3C and 3D for ^3H and ^{63}Ni , respectively. Under ^3H , the gain follows Klein's limit up to ≈ 14 keV, after which it strays away for both p-n and p-i-n junctions (Figure 3A). This whole behavior is explained by the fact that many carriers created by high-energy beta particles are generated beyond the junction, in the substrate. The energy dependence of the gain reveals that absorption occurs beyond the junction. The p-i-n junction slightly outperforms the p-n structure on both the gain and gain efficiency. It improves the collection of

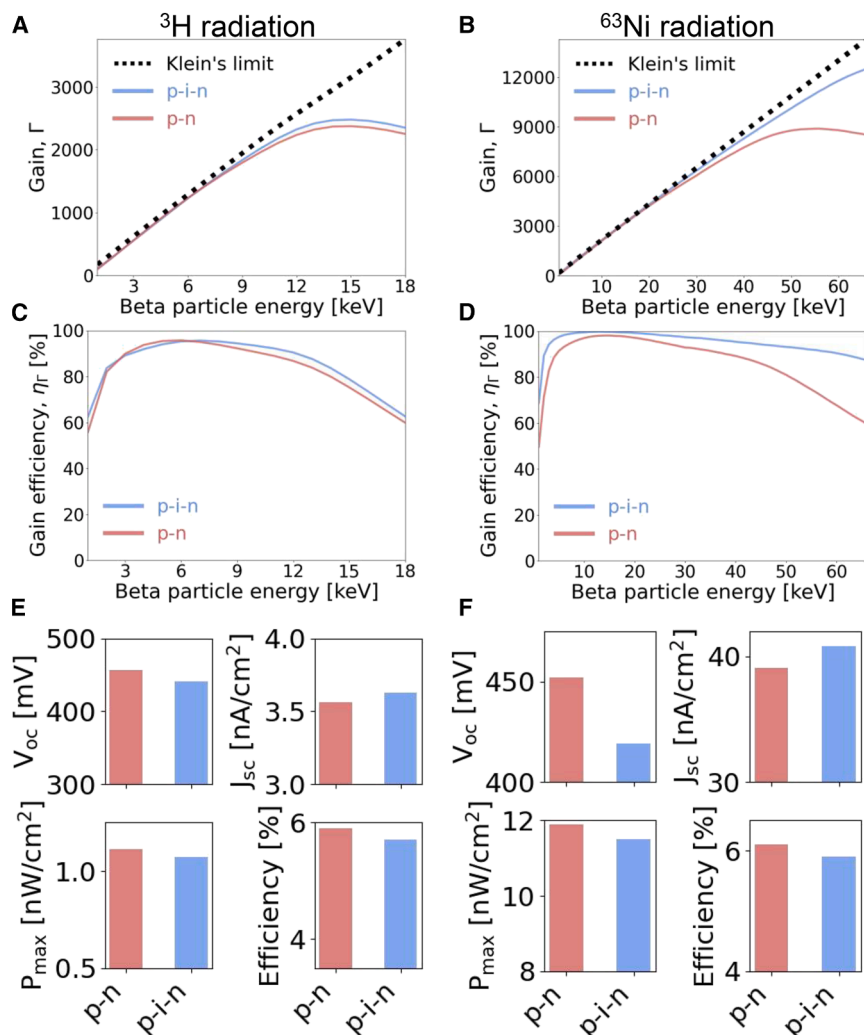


Figure 3. Betavoltaic cell gain, gain efficiency, and performance metrics

The left column presents the results under ^3H radiation, whereas the right column presents the results under ^{63}Ni radiation.

(A and B) Optimized betavoltaic cells gain under (A) ^3H and (B) ^{63}Ni radiation as a function of beta particle energy for each optimized design.

(C and D) Optimized betavoltaic cells gain efficiency under (C) ^3H and (D) ^{63}Ni radiation as a function of beta particle energy for each optimized design.

(E and F) Optimized betavoltaic cells performance metrics under (E) ^3H and (F) ^{63}Ni radiation for each design.

The main performance metrics (V_{oc} , J_{sc} , P_{max} , and efficiency) of the best p-n and p-i-n devices operating under ^3H are presented in Figure 3E. The efficiency is defined here as the ratio between the power density of the beta particles incident to the cell and the electrical power density generated by the device. The small improvement in current density generated by the p-i-n structure is reflected in the deviation of gain efficiencies (Figure 3C). However, due to a higher V_{oc} , the p-n structures slightly outperform the p-i-n devices in terms of power and efficiency. The figures of merit reveal that maximizing carrier collection does not result in maximizing the efficiency; the V_{oc} must be considered jointly.

Under ^{63}Ni , the gain closely follows Klein's limit at low energy, and it strays away at ≈ 45 keV for the p-n junction and at ≈ 60 keV for the p-i-n junction.

As carriers can be generated over $10\ \mu\text{m}$ deep under ^{63}Ni , efficient carrier collection represents a challenge. Therefore, p-i-n structures can improve carrier collection under this radioisotope, as they have a larger depletion region. This characteristic is also showcased in the gain efficiency, as the p-i-n device outperforms the p-n design over the full spectrum (Figure 3D).

Due to the deeper penetration of beta particles from ^{63}Ni than ^3H , devices must be designed more carefully to ensure carrier collection. Figure 3F presents the main performance metrics of the best devices operating under ^{63}Ni . Devices optimized for ^{63}Ni are an order of magnitude thicker than those optimized for ^3H . The design rules for ^{63}Ni are thus different than those for ^3H , as maximizing the current density is important. In other words, the figures of merit reveal that the current collection is important for ^{63}Ni betavoltaics, and the junction type has a larger impact than for ^3H . However, even if p-i-n structures maximize carrier collection, the p-n junction outperforms its p-i-n counterpart. This tradeoff between carrier collection and voltage is common for p-i-n architecture in photovoltaics, as well. The electric field that helps collect carriers also reduces the attainable V_{oc} . In the

carriers generated farther away from the junction. This is shown by the larger gain efficiency at low energy (< 3 keV) and at high energy (> 7 keV), as the carriers are generated closer to the surface and deeper in the heterostructure, respectively. The figures of merit reveal that adding an intrinsic GaAs layer in a betavoltaic cell operating under tritium improves carrier collection in these regions.

Figure 3C reveals a gain efficiency loss associated with low-energy beta particles. Low-energy beta particles generate carriers within the first tens of nanometers from the surface. They are therefore more susceptible to surface recombination, reducing the gain efficiency. Unlike in photovoltaics, it is challenging to design a high-band-gap window layer that reduces surface recombination while simultaneously being highly transparent to beta particles. This low gain efficiency at the front surface is also observed under ^{63}Ni (Figure 3D), as the challenge remains the same. This effect underlines the importance of the gain efficiency, as the energy dependence of the figure of merit can identify recombination losses on the front side of the device. The gain can not identify this loss mechanism.

Table 1. Betavoltaic figures of merit ranges, typical values, and their photovoltaic equivalent

Betavoltaic figures of merit	Value range	Typical values	Photovoltaic equivalent
Capture efficiency ($\eta_{\text{capture}}(\epsilon)$)	0%–100%	50%–90%	absorption factor
Gain ($\Gamma(\epsilon)$)	0 – $\Gamma_{\text{Klein}}(\epsilon)$	0–9,000 (^3H) 0–35,000 (^{63}Ni)	N/A
Gain efficiency ($\eta_{\text{r}}(\epsilon)$)	0%–100%	50%–99%	internal quantum efficiency

photovoltaic field, once material quality becomes large enough that diffusion lengths exceed absorption lengths, the best devices are p-n rather than p-i-n structures. Last, heterostructures approaching 10 μm can represent a challenge in epitaxy due to long deposition times. Therefore, a thinner structure represents an appealing choice from a fabrication standpoint. While p-n structures seem appealing for GaAs cells under ^3H and ^{63}Ni , it is worth pointing out that it may not be the case for all radioisotope-semiconductor combinations. Semiconductors with a different density, combined with radioisotopes with more energetic beta particles, could require a p-i-n structure to maximize power output. Furthermore, the edge of the betavoltaic cell can influence carrier recombination dynamics, thereby affecting overall device performance. These considerations underscore the importance of using energy-dependent figures of merit to accurately identify and quantify the sources of performance losses.

DISCUSSION

The capture efficiency, gain, and gain efficiency reveal many important design considerations for betavoltaics. The capture efficiency provides information on radioisotope and absorber material choice for maximizing energy transfer. Tritium is more affected by low energy (1–10 keV) backscattering and secondary electron losses than ^{63}Ni . Absorber materials with lower atomic numbers and lower densities enable a higher capture efficiency. This opens the path to metamaterial engineering to further minimize capture efficiency losses.

Gain and gain efficiency reveal that maximizing carrier collection is more important under ^{63}Ni . The lower gain efficiency at low beta particle energies reveals that the window layer must be designed so that it will limit parasitic absorption while providing good surface passivation. The optimization process tried to mitigate these losses by minimizing the thickness of the window layer down to 10 nm, matching the lower bound we allowed. The lower gain efficiency at high beta particle energy reveals two important mechanisms: (1) maximizing the V_{oc} requires omitting the absorption of carriers generated deeper under ^3H , and (2) bulk recombination limits carrier collections under ^{63}Ni .

Optimizing designs for betavoltaic cells requires careful consideration of the radioactive isotope, the junction structure, and the semiconductor materials. The capture efficiency, gain, and gain efficiency analyses untangle multiple complex relationships between these design considerations to identify the impor-

tant parameters under specific conditions. Table 1 summarizes all three figures of merit, their minimum and maximum values, their typical values, and their photovoltaic equivalent. The capture efficiency and gain efficiency are analogous to the absorption factor and the internal quantum efficiency in photovoltaics. The absorption factor and internal quantum efficiency being ubiquitous in many photovoltaic technologies suggests that these figures of merit will be useful in betavoltaics. The gain does not have a photovoltaic equivalent, as the multiplier effect is unique to betavoltaics. These figures of merit use physical characteristics universal to many technologies, enabling benchmarking between different betavoltaic system designs. The three figures of merit can be obtained experimentally with electron-beam-induced current measurements, facilitating design cycles between modeling and experimental work. While this work was performed on GaAs, GaN, and SiC semiconductors, it can readily be applied to other materials, such as perovskites, wide-band-gap oxides, diamond, or dye-sensitized cells.^{32–35}

METHODS

Numerical model

The betavoltaic device simulations were performed by combining three pieces of software: Monte Carlo simulation of electron trajectory in solids (CASINO), Radiation Ionization Converter to Carriers (RICC), and Sentaurus, described hereafter. Figure 4A shows the simulation process and its software as well as the associated schematic to illustrate the purpose of each software. The software CASINO^{36,37} performs Monte Carlo simulation of high-energy electron (>50 eV) trajectories in solids. CASINO is used to assess the energy density deposited ($e_{\text{transmitted}}(\epsilon, z)$) by beta radiation in the betavoltaic cell as a function of the beta particle energy (ϵ) and the depth (z) into the heterostructure. All simulated beta particles have a normal incidence. 10^6 electron trajectories are simulated for each beta particle energy to limit the relative error in energy deposition to 4.5%.³⁸ Simulations are performed in increments of 1 keV for the full ^3H and ^{63}Ni spectra, as illustrated in Figure 2.

The energy transfer from the beta particles to the betavoltaic cell leverages multiple mechanisms, as depicted in Figure 4B. Each beta particle has a gain effect, creating a cascade of secondary electrons through impact ionization. The secondary electrons can thermalize, becoming the carriers that will be collected by the device. The interaction between the beta particles and the betavoltaic cell will generate high-energy photons that can also generate electron-hole pairs. These stochastic events happen in succession until each beta particle or secondary electron escapes the device or thermalizes. Considering the randomness of the process, one can define an average energy for which an electron-hole pair is generated through beta particle impact ionization. Previous work by Klein²⁸ proposed the following empirical relationship (Equation 1):

$$\epsilon = 2.8E_g + 0.5 \text{ (eV)} \quad (\text{Equation 1})$$

In Equation 1, ϵ is the radiation-ionization energy, or the average energy required to form an electron-hole pair from a beta particle

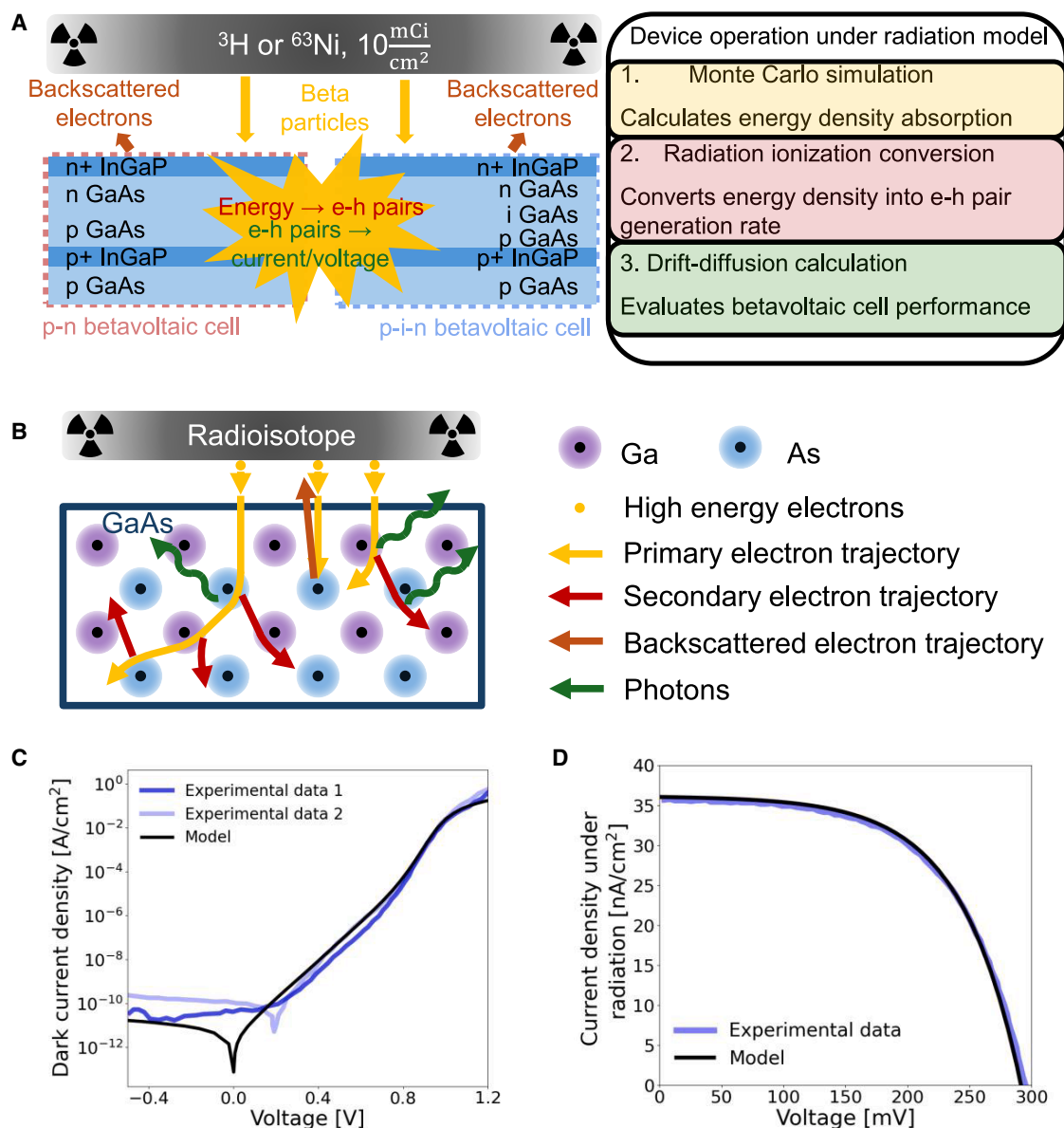


Figure 4. Simulation methods, betavoltaic conversion mechanism, and model validation

(A) Schematics depicting the numerical methods used here to model betavoltaic cells.

(B) Schematic illustrating energy transfer from beta particles in GaAs. Beta particles can generate secondary electrons, photons, and phonons. Beta particles can also be backscattered.

(C) Dark I-V characteristics of experimental data obtained by Schmieder et al.³⁹ and reproduced numerically in this work to validate and calibrate the material parameters.

(D) I-V characteristics of a betavoltaic cell operating under beta radiation. The experimental data were obtained by Chen et al.⁴⁰ and were reproduced numerically in this work to validate and calibrate the models used to calculate betavoltaic conversion.

impact ionization; E_g is the band gap of the semiconductor material constituting the betavoltaic cell.

The next calculation step consists of converting the energy density profile ($e_{\text{transmitted}}(\mathcal{E}, z)$) into an electron-hole pair generation rate profile ($G(\mathcal{E}, z)$). A custom software, RICC, performs this calculation using the empirical Equation 1. The electron-hole pair generation rate then depends on the energy density transmitted to the heterostructure ($e_{\text{transmitted}}(\mathcal{E}, z)$) as a function

of the beta particle energy ($\mathcal{E}$) and the depth (z). The generation rate can therefore be written as

$$G(\mathcal{E}, z) = \frac{e_{\text{transmitted}}(\mathcal{E}, z)}{\mathcal{E}}, \quad (\text{Equation 2})$$

where $G(\mathcal{E}, z)$ is the generation rate created by an electron of energy $\mathcal{E}$ at a depth z . By weighting the energy with the beta energy

probability density ($\frac{dN}{d\mathcal{E}}$) and integrating the product over the fitted radioisotope emission spectrum, for each 1 keV increment, the electron-hole pair generation rate created by a radioisotope is

$$G_{\text{radioisotope}}(z) = \int_{\text{radioisotope spectrum}} \frac{dN(\mathcal{E})}{d\mathcal{E}} \frac{e_{\text{transmitted}}(\mathcal{E}, z)}{\mathcal{E}} d\mathcal{E}, \quad (\text{Equation 3})$$

Additional losses are considered to complete the model, such as radioisotope self absorption³⁸ and air absorption if the radioisotope is not in direct contact with the betavoltaic cell.

The electron-hole generation rate profiles are sent to the commercial software Synopsys technology computer-aided design (TCAD) Sentaurus (S-2021.06). The electrical properties of the betavoltaic devices are assessed by solving Poisson, drift, and diffusion equations in 1 dimension with the carrier generation rate as calculated from RICC. The minimal mesh size is 1 nm. As shown in Figure 4A, the studied betavoltaic cells are GaAs p-n and p-i-n junctions. They are cladded with an InGaP window and an InGaP back surface field. A GaAs substrate is assumed. Doping-dependent mobilities were calculated using values reported in the literature.⁴¹ Parameters for band gap, effective masses, radiative recombination, and Auger recombinations were obtained from the literature.⁴²

The betavoltaic cell modeling platform combining CASINO, RICC, and Sentaurus was calibrated and validated using experimental data from the literature. The first step of the validation consists of reproducing a dark current-voltage (I-V) measurement taken from the literature³⁹ to validate the material properties. Figure 4C compares the experimental results of two samples by Schmieder et al.³⁹ and our simulation results. A Shockley-Read-Hall (SRH) lifetime of 30 ns was considered to validate the model, which is in agreement with the values reported by the authors.³⁹ Our model agrees well with the experimental data, which suggests that the material parameters used in the Poisson, drift, and diffusion calculations are well defined. The second validation step consists of numerically reproducing the experimental results of a betavoltaic cell operating under beta radiation to validate the models of CASINO and RICC. Figure 4D illustrates the experimental results from Chen et al.⁴⁰ obtained under a ⁶³Ni source with an activity of 10 $\frac{\text{mCi}}{\text{cm}^2}$ and the results reproduced by the numerical model. The experimental data could be reproduced within 1% with our model by assuming that the beta radiation source had an empirical self-absorption coefficient of 89% and was placed 1 mm away from the cell. The agreement between the experimental data and our model suggests that the CASINO and RICC models reproduce the betavoltaic conversion mechanisms numerically with high fidelity. The same source activity (10 $\frac{\text{mCi}}{\text{cm}^2}$) was used for this work.

From the simulation results, we calculate the V_{oc} , J_{sc} , P_{max} , and efficiency. The V_{oc} corresponds to the voltage generated by the device under open-circuit conditions. The J_{sc} is the current density generated by the cell while it is under short-circuit conditions. The P_{max} corresponds to the product of the voltage and current density combination for which their product is maximal. The efficiency is the ratio between the P_{max} generated by the cell to the incident power density from the radioisotope onto the device.

An in-house high-dimensionality particle swarm algorithm was used to find the optimal layer thicknesses and doping levels. The objective function has one goal, which is to maximize the power density generated by the cell. The algorithm is adapted from the particle swarm optimization algorithm,⁴³ with the main modification being repositioning of the particles after a specific number of iterations⁴⁴ to improve robustness in high-dimension calculations. The emitter and base thickness lower bounds were set to 10 and 200 nm, respectively. The lower bounds for the non-intentionally doped layer were set to 10 nm and 1 μm for ³H and ⁶³Ni, respectively. For all three layers (n, i, and p), the thickness upper bounds were 3 and 20 μm for ³H and ⁶³Ni, respectively. The emitter and base doping level bounds were set to 10^{16} and 7×10^{18} . These values were chosen based on the generation rate profile of each radioisotope (Figures 2C and 2D) as well as epitaxial growth limitations. The initial parameters were obtained randomly within the bounds. We used 120 starting parameter sets, and the optimizer investigated the parameter space over 50 iterations. 50 iterations were enough to obtain convergence, as the optimal structure was typically found upon reaching the ≈ 40 th iteration.

Figures of merit

The generation rate is affected by the device's efficacy in capturing beta particle energy. We define the first figure of merit, the capture efficiency, as the ratio between the energy transmitted to the cell and the energy incident to the betavoltaic cell as a function of beta particle energy:

$$\eta_{\text{capture}}(\mathcal{E}) = \frac{\int_{\text{depth}} e_{\text{transmitted}}(\mathcal{E}, z) dz}{E_{\text{incident}}(\mathcal{E})}. \quad (\text{Equation 4})$$

In this equation, $\eta_{\text{capture}}(\mathcal{E})$ is the capture efficiency (unitless) for a beta particle of energy $\mathcal{E}$, $e_{\text{transmitted}}(\mathcal{E}, z)$ is the energy density (eVnm^{-1}) transmitted to the betavoltaic cell, and $E_{\text{incident}}(\mathcal{E})$ is the energy (eV) incident to the betavoltaic cell. While it is similar to the coupling efficiency,³ the figure of merit proposed here identifies losses in different regions of the radioisotope spectrum. It is analogous to the absorption factor in photovoltaics.⁴⁵

A single radioisotopic beta particle can generate many electron-hole pairs through impact ionization, since beta decay emission energies are orders of magnitude higher than the radiation ionization energy. Betavoltaic devices present a gain effect, or the carrier generation amplification relative to incident particle flux, when converting high-energy beta particles into electron-hole pairs. The current density that the device can collect is much higher than the beta particle flux. We define the second figure of merit, the device gain ($\Gamma(\mathcal{E})$), as the ratio between the short-circuit current density ($J_{\text{sc}}(\mathcal{E})$) to absorbed beta particle flux:

$$\Gamma(\mathcal{E}) = \frac{J_{\text{sc}}(\mathcal{E})}{qA_{\text{Rad}}(\mathcal{E})(1 - R(\mathcal{E}))}. \quad (\text{Equation 5})$$

In Equation 5, $\Gamma(\mathcal{E})$ is the gain (unitless) created by a beta particle of energy $\mathcal{E}$, $J_{\text{sc}}(\mathcal{E})$ is the short-circuit current density (Acm^{-2}) generated by beta particles of energy $\mathcal{E}$, q is the elementary

charge (C), $A_{\text{Rad}}(\mathcal{E})$ is the beta particle flux ($\text{cm}^{-2}\text{s}^{-1}$) of energy $\mathcal{E}$ emitted by the radioisotope, and $R(\mathcal{E})$ is the fraction of beta particles of energy $\mathcal{E}$ that was not transmitted to the betavoltaic cell (unitless). The gain (Γ) has a theoretical limit when all of the generated carriers are collected. We call this limit Klein's limit ($\Gamma_{\text{Klein}}(\mathcal{E})$), which is

$$\Gamma_{\text{Klein}}(\mathcal{E}) = \frac{\int_{\text{depth}} G(\mathcal{E}, z) dz}{A_{\text{Rad}}(\mathcal{E})(1 - R(\mathcal{E}))}. \quad (\text{Equation 6})$$

In this equation, $G(\mathcal{E}, z)$ is the generation rate created by beta particles of energy $\mathcal{E}$ at a depth z .

We define the third figure of merit, the gain efficiency ($\eta_{\Gamma}(\mathcal{E})$), as the ratio between the gain and Klein's limit:

$$\eta_{\Gamma}(\mathcal{E}) = \frac{\Gamma(\mathcal{E})}{\Gamma_{\text{Klein}}(\mathcal{E})}. \quad (\text{Equation 7})$$

This performance parameter is unitless and is analogous to the internal quantum efficiency for solar cells. A hypothetical gain efficiency of 100% means that all electron-hole pairs generated from beta particles with energy $\mathcal{E}$ are collected. A gain efficiency of less than 100% means that some electron-hole pairs are generated but not successfully collected due to radiative, Auger, or SRH recombination. The gain efficiency parameter identifies the origin of current losses in betavoltaic cells as a function of the beta particle energy. It indicates the depth where carriers are generated in the heterostructure but not successfully collected.

RESOURCE AVAILABILITY

Lead contact

Requests for further information and resources should be directed to the lead contact, Mathieu de Lafontaine (mdelafon@uottawa.ca).

Materials availability

This study did not generate new, unique materials.

Data and code availability

- All data reported in this paper will be shared by the lead contact upon request.
- The software CASINO is available at <https://casino.espaceweb.usherbrooke.ca/>. The TCAD Sentaurus project and Python scripts used for the simulations within this paper are available at Zenodo (<https://doi.org/10.5281/zenodo.15856514>).
- Any additional information required is available from the [lead contact](#) upon request.

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AUTHOR CONTRIBUTIONS

Conceptualization, M.d.L., J.P.D.C., J.P., B.E., and H.F.; methodology, M.d.L., C.S., R.F.H.H., G.P.F., and J.P.D.C.; investigation, M.d.L. and C.S.; writing – original draft, M.d.L.; writing – review & editing, M.d.L., R.F.H., G.P.F., J.P.D.

C., J.J.K., and K.H.; funding acquisition, M.d.L., J.P.D.C., J.P., B.E., H.F., J.J.K., and K.H.; resources, M.d.L., C.S., R.F.H.H., G.P.F., J.P.D.C., J.P., B.E., H.F., J.J.K., and K.H.; supervision, J.P.D.C., J.P., B.E., H.F., J.J.K., and K.H.

DECLARATION OF INTERESTS

K.H. is a co-founder and president of Enurgen. J.P., B.E., and H.F. are employees of the Canadian Nuclear Laboratories, the contractor responsible to manage and operate the Atomic Energy of Canada Limited sites and facilities across the country. M.d.L., J.P.D.C., and K.H. have a patent application: Radioisotope power converter device architectures, US Patent Application 18/740,623, June 12, 2024.

DECLARATION OF GENERATIVE AI AND AI-ASSISTED TECHNOLOGIES IN THE WRITING PROCESS

The authors used a particle swarm optimization algorithm to rapidly survey a high-dimensionality parameter space to find the maximum power output of betavoltaic cells. GitHub Copilot was used to accelerate writing the code. Grammarly was used to proofread the manuscript.

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