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# **Design optimization of GaAs betavoltaic batteries**

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### Abstract

GaAs junctions are designed and fabricated for betavoltaic batteries. The design is optimized according to the characteristics of GaAs interface states and the diffusion length in the depletion region of GaAs carriers. Under an illumination of 10 mCi cm<sup>-2</sup> <sup>63</sup>Ni, the open circuit voltage of the optimized batteries is about ~0.3 V. It is found that the GaAs interface states induce depletion layers on P-type GaAs surfaces. The depletion layer along the P<sup>+</sup>PN<sup>+</sup> junction edge isolates the perimeter surface from the bulk junction, which tends to significantly reduce the battery dark current and leads to a high open circuit voltage. The short circuit current density of the optimized junction is about 28 nA cm<sup>-2</sup>, which indicates a carrier diffusion length of less than 1  $\mu$ m. The overall results show that multi-layer P<sup>+</sup>PN<sup>+</sup> junctions are the preferred structures for GaAs betavoltaic battery design.

(Some figures in this article are in colour only in the electronic version)

Betavoltaic batteries are attractive candidates for micro-power sources because of their long lifetime (tens of years) and super high energy density (ten times higher than that of lithium ion batteries), which have attracted increasing research attention in recent years [1-9]. At present the output power (in the order of nW) and energy conversion efficiency (<8%) are very low, which significantly limits the applications of the batteries. Many wide bandgap semiconductors such as SiC, 4H SiC and InGaP [1-3] have been investigated for their high resistance of irradiation and great potential for achieving large open circuit voltage to improve the output power and energy conversion efficiency. However, wide bandgap semiconductors grown with current technology show poor reproducibility and stability. For example,  $500 \times 500 \,\mu m$ 4HSiC betavoltaic batteries [2] show a typical leakage current density of  $10^{-12}$  A cm<sup>-2</sup>.

In this study, GaAs and <sup>63</sup>Ni source are selected as the material system for a high-performance betavoltaic battery. GaAs can be grown with very high crystal quality, which has been widely employed in the semiconductor industry, such as in optoelectronic devices and photovoltaic cells. GaAs shows high irradiation resistance (threshold 225 keV

[10]), which makes it work fine under the irradiation of  $^{147}$ Pm.

To obtain a thicker depletion region and better ohmic contact, PIN junctions are widely used in betavoltaic batteries [1-3]. In this paper, four types of PIN junctions, P<sup>+</sup>PN<sup>+</sup>, N<sup>+</sup>NP<sup>+</sup>, P<sup>+</sup>NN<sup>+</sup> and N<sup>+</sup>PP<sup>+</sup> are designed to study the impacts of interface states on the characteristics of batteries. P<sup>+</sup>PN<sup>+</sup> junctions with different depletion region thicknesses are designed to evaluate the carrier diffusion length in the depletion region.

The leakage current of a GaAs PN junction consists of two parts: (1) the bulk junction leakage current; (2) the perimeter recombination current of the perimeter surface that intersects the depletion layer [11, 12]. Typically, the perimeter recombination current is the main source of leakage current and it increases with the density of interface states.

However, on the other hand, GaAs interface state density is very high  $(10^{12}-10^{14} \text{ cm}^{-3} \text{ eV}^{-1})$  and the interface potential is pinned at 0.8 eV [13]. Accumulation layers and depletion layers are formed on N-type and P-type GaAs surfaces, respectively, as indicated by the drift of *C*–*V* curves along the voltage axis of metal–SiO<sub>2</sub>–GaAs structures [14]. Due



**Figure 1.** Equivalent circuit for the isolation effect.  $R_d$  is the resistance of the PDL induced by the interface states.  $R_p$  is the parallel resistance of the junction caused by the interface states.

to high resistances, the depletion layers around a  $P^+PN^+$ junction's perimeter surface isolate the perimeter surface from the bulk junction and significantly decrease the  $P^+PN^+$ junction's leakage current. The isolation effect increases with the density of interface states. As shown in figure 1, an equivalent circuit is used to explain the isolation effect.

The principle cannot be validated by simply comparing the leakage current of  $P^+PN^+$  GaAs junctions with high and low interface states, as explained earlier. In the following experiments, the comparisons between  $P^+PN^+$  (with isolation effect) and  $N^+NP^+$  (without isolation effect) junctions demonstrate the isolation effect of the perimeter depletion layers (PDLs) induced by interface states in which two kinds of junctions have similar bulk junction leakage currents and perimeter recombination currents.

 $P^+PN^+$ ,  $N^+NP^+$ ,  $P^+NN^+$  and  $N^+PP^+$  junctions are fabricated, and the schematic structures are shown in figure 2. The heavily doped top layer and the shallowly doped layer are the active regions of a battery. In total, 160 prototype batteries (40 for each type of  $P^+PN^+$ ,  $N^+NP^+$ ,  $P^+NN^+$  and  $N^+PP^+$ ) are fabricated to test the output stability and reproducibility.

GaAs epilayers are grown by molecular beam epitaxy (MBE) at 580 °C and a growth rate of 1  $\mu$ m h<sup>-1</sup> on N-type and P-type GaAs substrates with a doping concentration of 1 × 10<sup>18</sup> cm<sup>-3</sup>. Ohmic contacts are made by thermal evaporation. For the contacts on N-type GaAs, 500 Å Ni, 250 Å Ge and 1  $\mu$ m Au were deposited subsequently, and for the contacts on P-type GaAs, 100 Å Ni, 150 Å Pt and 1  $\mu$ m Au were deposited. A SiO<sub>2</sub> passivation layer of 500 Å was grown by PECVD at 300 °C. Battery areas are designed as 5 × 5 mm<sup>2</sup>. <sup>63</sup>Ni with an activity of 10 mCi cm<sup>-2</sup> is used as the beta source.

Metal layers can introduce significant backscattering of electrons. Hence, in a 4HSiC betavoltaic battery even a thin layer of Ni, 100 nm, can cause a 25% reduction in current multiplication when illuminated by 17 keV electron beam [15]. Therefore, in our design the junction is prepared with a ring electrode contact to minimize shadowing of the radiation by the metal layer. Reducing electrode area may introduce series resistance, in the range of tens to hundreds of ohms, to the junction, but it has little impact on the batteries' output characteristics for the batteries' low output currents ( $\sim$ nA). No significant changes are observed in the measured beta *I*–*V* characteristics when the junctions are in series with resistances of 100, 300 or 500  $\Omega$ .

The leakage current of the GaAs PN junction can be approximately expressed by [11, 12, 16]

$$J = J_{\rm b} + J_{\rm s} = \int_0^{W_{\rm D}} q U \,\mathrm{d}x + q P \int_0^{W_{\rm D}} R \,\mathrm{d}x, \qquad (1)$$

where  $W_D$  is the thickness of the built-in electron field, U is the recombination rate, R is the surface recombination rate which is increased with the interface state density, q is the elementary charge and P is the length of the junction perimeter.

The uniform short circuit currents of the aforementioned junctions indicate uniform crystal qualities of the bulk junctions, which implies similar recombination rates in the built-in electric field. Hence, the bulk junction leakage currents are close to each other in these junctions. The high interface density on the GaAs surface shows that the surface recombination rates on N-type and P-type GaAs are similar to each other. Hence the perimeter junction leakage currents are also close to each other in the P<sup>+</sup>PN<sup>+</sup>, N<sup>+</sup>NP<sup>+</sup>, P<sup>+</sup>NN<sup>+</sup> and N<sup>+</sup>PP<sup>+</sup> junctions. So, the differences in open circuit voltages and leakage currents in figure 2 are caused by the isolation effect of the PDLs.

The leakage currents of the junctions can be extracted from the forward active region of the I-V curves The relationship of the leakage curin figure 2. rents is  $I_0(P^+PN^+, \sim 10^{-11} \text{ A}) \ll I_0(N^+PP^+, \sim 10^{-9}) <$  $I_0(P^+NN^+, \sim 10^{-9} \text{ A}) < I_0(N^+NP^+, \sim 10^{-8} \text{ A})$ . As shown in figure 4, the more the built-in electric field perimeter (the heavily doped top layer and the shallowly doped layer) covered by PDLs, the stronger the isolation effect, and hence lower the leakage current. Hence, P+PN+ junction is preferred for GaAs betavoltaic batteries. As the built-in electric field perimeter is not fully covered by PDLs, the P<sup>+</sup>NN<sup>+</sup> and N<sup>+</sup>PP<sup>+</sup> junction leakage currents are dominated by the perimeter recombination currents and close to those of the N+NP+ junctions, which confirm that the surface recombination currents are close to each other in the P<sup>+</sup>PN<sup>+</sup>, N<sup>+</sup>NP<sup>+</sup>, P<sup>+</sup>NN<sup>+</sup> and N<sup>+</sup>PP<sup>+</sup> junctions and that the different open circuit voltages and leakage currents of the junctions are caused by the isolation effect.

The typical beta I-V curves of junctions 5 and 6 are similar to that of junction 4. Hence, the short circuit currents of these junctions are similar to each other. This implies that the carrier diffusion length in the depletion region may be shorter than 1  $\mu$ m, and that increasing the depletion region thickness has no contribution to the short current when the depletion region thickness is larger than the carriers' diffusion length.

The carrier diffusion length in the depletion region can be evaluated based on the comparisons between the measured currents and the ideal short circuit currents. The ideal short circuit current,  $I_{id}$ , can be calculated as

$$I_{\rm id} = \frac{E(R)}{\varepsilon} \times q \tag{2}$$



Figure 2. Schematic structures of the GaAs junctions.



**Figure 3.** The typical beta I-V characteristics of the GaAs junctions.

with

$$E(R) = A_{c} \times \left\{ \int_{0}^{E_{R}} P(E) dE + \int_{E_{R}}^{E_{max}} P(E) \left( E^{-1} \times \int_{0}^{R_{E}} \frac{dE}{dx} dx \right) dE \right\}, \quad (3)$$

where  $A_c$  is the activity of <sup>63</sup>Ni, E(R) is the energy deposited by <sup>63</sup>Ni in the GaAs layer within  $R \ \mu m$ ,  $\varepsilon$  is the mean electron– hole pair ionization energy of GaAs which is 4.6 eV, a widely used value [17], P(E) is the energy spectrum of <sup>63</sup>Ni,  $E_R$  is the energy of a beta particle whose penetration depth in GaAs is  $R \ \mu m$ ,  $E_{max}$  is the maximum energy of the <sup>63</sup>Ni energy spectrum, E is the kinetic energy of beta particles,  $R_E$  is the penetration depth of a beta particle with kinetic energy E [18] and dE/dx is the stopping energy of GaAs. It can be calculated by different ways such as the continuous slowingdown approximation [19] and the models of Kanaya–Okayama (K–O) [15], Wittry–Kyser [17] and Everhart–Hoff [20]. In this paper, the K–O model is used. The P(E),  $R_E$  and dE/dx can be expressed as follows:

$$P(E) = \frac{g_{\rm GT}^2 |M_{\rm GT}|^2}{\pi^3 c^3 \hbar^7} F(Z, E) (E_m - E)^2 mE,$$
(4)

$$R_E = (2.67 \times 10^{-2}) \frac{AE^{5/3}}{\rho Z^{8/9}} \left(\frac{1 + E/2m_0 c^2}{1 + E/m_0 c^2}\right)^{5/3},$$
(5)

$$\frac{dE}{dx} = \frac{\rho}{E} \frac{\gamma}{(1-y^2)\rho R} \exp\left(-\frac{\gamma y}{1-y}\right) \times \left\{1 + \frac{6 \times 1.9}{5} \exp\left(-\frac{0.9\gamma y}{1-y}\right) \times \left(\frac{1}{2^{5/6}} - (1-y)^{5/6}\right)\right\},$$
(6)

$$y = x/R_{\rm K-O},\tag{7}$$

$$\gamma = 0.187 Z^{2/3},\tag{8}$$

where  $g_{\text{GT}}$  is a constant,  $M_{\text{GT}}$  is the nuclear matrix, F(Z, E) is the Coulomb-modified coefficient, *m* is the electron mass, *c* is the velocity of light,  $\hbar$  is the Planck constant, *Z* is the nuclear charge number,  $\rho$  is the GaAs density and *A* is the atom weight.

The energy deposited in GaAs, E(R), and the ideal short circuit current,  $I_{id}$ , versus built-in electric field thickness is plotted in figure 5. Within the  $1 \,\mu$ m depletion region the curve in figure 5 can be seen as a line approximately, and this means that the deposited energy and the induced electronhole pairs distribute uniformly along the thickness direction. As for junction 4, the measured short circuit current density,  $28 \text{ nA cm}^{-2}$ , is about half of the ideal short circuit current density, which means only half of the electron-hole pairs in the built-in electric field are collected causing the short circuit current. Hence, it can be concluded that the carrier diffusion length in the built-in electric field is about 0.5  $\mu$ m, one half of the electric field thickness of junction 4. So a multi-junction structure is preferred for GaAs betavoltaic batteries, and the number of junctions should be 6-10 when the isotope source is <sup>63</sup>Ni.



Figure 4. Schematic structures of PDLs.



Figure 5. Ideal short circuit current density and the energy deposited in GaAs versus the built-in electric field thickness.

In summary, P<sup>+</sup>PN<sup>+</sup>, N<sup>+</sup>NP<sup>+</sup>, P<sup>+</sup>NN<sup>+</sup> and N<sup>+</sup>PP<sup>+</sup> GaAs junctions passivated by SiO<sub>2</sub> are fabricated. Interface states induce depletion layers on P-type GaAs surfaces and the depletion layers along the P<sup>+</sup>PN<sup>+</sup> junction edges isolate perimeter junctions from the bulk junctions, which tends to significantly reduce the battery dark currents and then leads to a higher open circuit voltage than the other junctions. The carrier diffusion length in the built-in electric field is about  $0.5 \,\mu$ m, which is evaluated based on the comparisons between the measured currents and the calculated short currents. Hence under <sup>63</sup>Ni radiation, a multi-P<sup>+</sup>PN<sup>+</sup> junction (6–10 junctions) is the preferred choice for GaAs betavoltaic batteries.

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