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Modeling of betavoltaic cells GaN using a Monte Carlo calculation

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In this study, we use a Monte Carlo calculation code to simulate the concentration of electron-hole pairs generated of each point in the solid targets under a bombardment of Ni-63 source for betavoltaic cells; this model is reported to be an accurate representation of electron interaction.From this simulation we can obtain the distribution of electron-hole pairs generated in GaN/GaN junction as a function of the depth, this distribution allowed us to find the concentrations of minority carriers excess depending on the thickness, which can represent as function and inject into the continuity equations for determine the diffusion current and then the characteristics of betavoltaic chosen. The model has been tested for Ni-63/GaN/GaN structure, with energy 17 KeV.

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1. Introduction

The betavoltaic cells is direct conversion energy from isotope decay (beta particles, alpha particles) into electric power[1]. It's became a promising micro-power sources for many application such as, sensors in remote location, in equipment which consumes low energies but in the long term, as is the case in the components used in the cosmology which require long term energy and in other military applications etc ... [2].

In our study we are interested in the interaction of electron with matter for the creation pairs of electrons holes. Several Monte Carlo simulation models are proposed, based on different approaches to treatment electron scattering (elastic and inelastic). In this work we use a Monte Carlo method to calculate the concentration of the electro-hole pairs generated after a bombardment of structure (semiconductor) with an electron beam, as it was found in the CdS [3] using the same code and applying for GaN, this concentration of electron-hole pairs in matter (Gaussian form), allowed us to calculate the current that can be generated in a P-N junction betavoltaic. Our study consists to find the current generated without making the approximation of the dead zone, in order to take into account the gradient of minority carriers generated by the source Ni-63.

2. Model

The present Monte Carlo simulation of electron trajectories penetrating a sample is based on a description of beam electron scattering processes, it necessary determination of values of physical quantities such as step length, scattering angle, energy loss, and so forth, in a particular scattering event.

During the trajectory of the electron in a semiconductor, the electron loses its energy, between two collisions there is always a loss of energy, the process of energy deposition after the

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shock depends on the nature of the elastic or inelastic shock, in the case of the elastic shock there is no loss of energy, in the case of an inelastic shock there will be a deposit of energy given to the crystal to generate electron-hole pairs, the phenomenon giving the nature of the shock is modeled by a random number R which takes random values between 0 and 1, according to R the angle is determined, each electron travels a small distance S in straight line between random scattering events (elastic collision or inelastic). The step length S is derived from[4]:

$$S = -\lambda \ln(R) \tag{1}$$

λ: is the mean free path, can be obtain from the total scattering cross section as:

$$\lambda_m = \frac{A}{N_A \rho \sigma} \tag{2}$$

σ is the total scattering cross section is given by[5]:

$$\sigma = 5.21 \times 10^{-21} \frac{Z^2}{E^2} \frac{4\pi\lambda_c\left(1-e^{-\beta\sqrt{E}}\right)}{\delta(\delta+1)} \left(\frac{E+m_0c^2}{E+2\times m_0c^2}\right)^2 \tag{3}$$

where δ is a screening parameter given by:

$$\delta = (3.4 \times 10^{-3}) \frac{10^{0.67}}{E} \tag{4}$$

λ_c and β are constants for a given element,

$$\lambda_c = 1.162 + 1.28 \times 10^{-2} Z$$

$$\beta = \frac{26.42}{Z^{1.24}}$$

The angle α for particular scattering event can be obtained from the probability by the relationship[4]:

$$\cos\alpha = 1 - \frac{2\delta R}{1+\delta-R} \tag{5}$$

The azimuthal angle θ is given by:

$$\theta = (1 - 2R_1)\pi \tag{6}$$

R_1 is another random number uniformly distributed between 0 and 1.
θ is angle uniformly distributed between $-\pi$ and $+\pi$

We suppose that the incident electron arrives parallel to the normal of the surface of the matter.

If $\theta > \frac{\pi}{2}$ or $\theta < -\frac{\pi}{2}$ the electron leaves the matter and will be supposed to be backscattered electron, only angles between $-\frac{\pi}{2}$ and $\frac{\pi}{2}$ enter the matter.

In the next step we determine the amount of energy loss the equation, after each collision the electron lost energy, the rate of loss energy used in this simulation given by [5]:

$$\frac{dE}{dS} = -7.85 \times 10^4 \frac{\rho Z}{AE} \ln\left(\frac{1.166(E+kJ)}{J}\right) \text{(KeV/cm)} \tag{7}$$

After inelastic collision the electron lost also energy E_{e-h} to generate one pair electron-hole. The electron-hole pair creation energy can be taken [6]:

$$E_{e-h} = 2.73E_g + 0.5 \tag{8}$$

We are interested in the generation of electron-hole pairs produced during the collision of the incident electrons with the atoms of the semiconductor. After each inelastic collision the electrons lose E_{e-h} energy to produce an electron-hole pair, until the energy falls below the value: $3 \times E_g$. To simplify the calculation two dimensions, x and z are considered, which can be generated in three dimensions and that the concentration along the z axis does not change since x and y are symmetrical.

3. Results and discussion

To understand electron beam interaction phenomenon, we have to understand electron penetration into matter, it is necessary to know information about the number of electron and energy, the stopping range finding by Kanaya and Okayama relationship [7]:

$$R = \frac{2.76\times10^{-6}}{\rho}\frac{A}{Z^{8/9}}(E_0)^{5/3}: \tag{9}$$

In our model, we calculate the stopping range of the semiconductor used and we compare with the stopping range finding by Kanaya and Okayama to validate the results found by the proposed method.

To calculate the stopping range proposed by our model we take the average penetration of 100 electrons

$$R = \frac{\sum_{i=1}^{n} r_{max}}{n} \tag{10}$$

where n is the number of incident electron in our case equal 100.

r_{max} is the maximum distance of the electron travels in the matter before losing all of its energy and stopping.

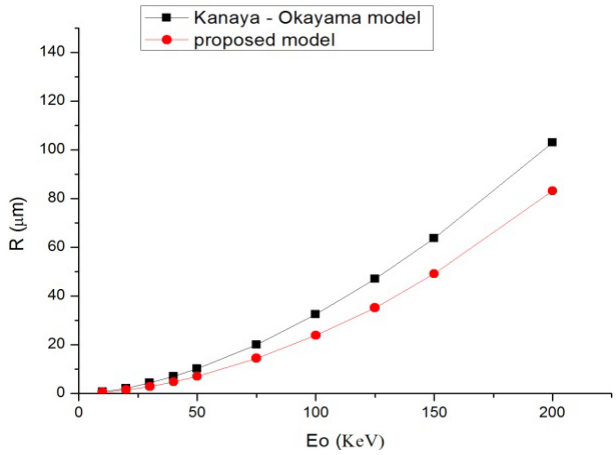

Fig. 1. Stopping range of electrons for GaN as function of acceleration energy.

We notice that the depth of penetration obtained in our model is in good agreement with Kanaya and Okayama models for low energies.

We calculate the energy variation (the energy loss), If (E > E_{e-h}) ,there is formation of an electron-hole pair, The sample is divided by several zones. At each zone, quantities of electron-hole pairs are generated, is the profile of distribution of electron-hole pairs generated depending of the thickness (z).

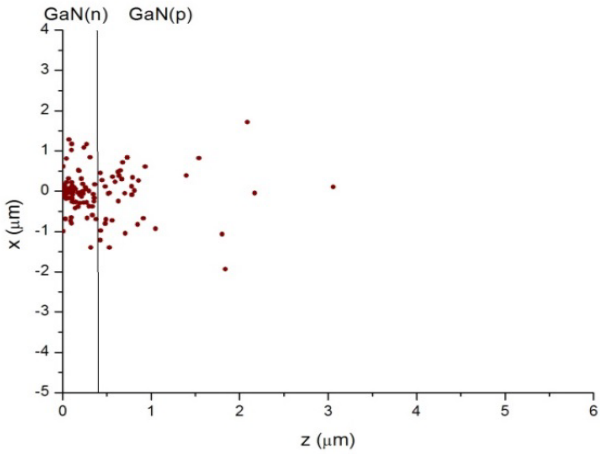

Fig. 2. The distribution of electron-hole pairs generated as a function of depth in GaN for an acceleration energy 17 KeV.

We notice that most of the concentration of electron hole generated is just below the surface.

The variation of the minority charge carriers Δn (x) in the p-type semiconductor and Δp (x) in the n-type semiconductor is calculated as a function of the depth in the (fig.3.) for energies 17 KeV.

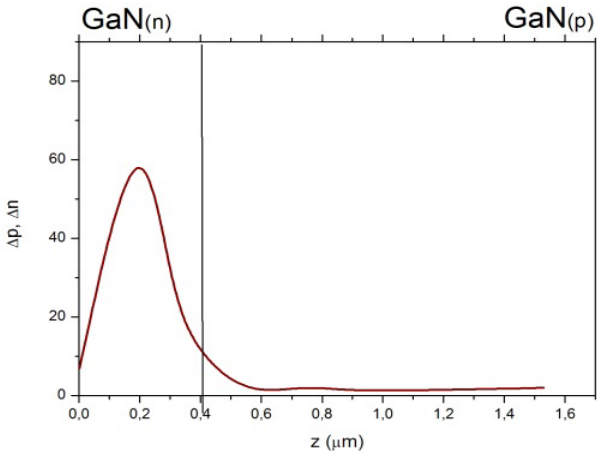

Fig. 3. The distribution of the concentration of electron-hole pairs generated by inelastic collisions of the incident electron in GaN/GaN.

Using the distribution of the concentration of EHPs generated of the incident electron in the structure to define the function G_{ph} of the concentration EHPs generated (minority carriers' excess depending on the thickness (x)).

$$G_{ph} = ae^{-(\frac{x-b}{c})^2} \quad (11)$$

where: a,b,c are constants for each cells present in (Table I):

Table 1. Fit function G_{ph} constants for GaN cells.

Incident energy (KeV)	GaN		
	a	b	c
17	82.398	0.0017919	0.0081372

To estimate the current flowing through the junction we have to solve the continuity equations, taking into account the function G_{ph}, in order to find the concentrations of the minority charge carriers (Δn , Δp) of the carriers on either side in the ZCE.

We simulated GaN/ GaN based betavoltaic cell, the parameter for GaN/ GaN cells used in our simulation are grouped in the following table:

Table 2. The parameters of GaN/GaN.

	$E_g\ (eV)$	$N_d\ cm^{-3}$	$N_a cm^{-3}$	n type thickness	type thickness
$GaN_{(n)}$	3.44	10^{19}	--	$0.4\ \mu m$	--
$GaN_{(p)}$	3.44	--	10^{17}	--	$2\ \mu m$

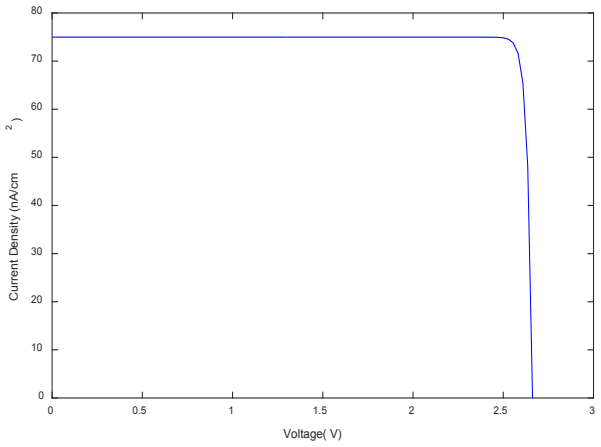

Fig. 4. Current Density voltage for GaN/GaN.

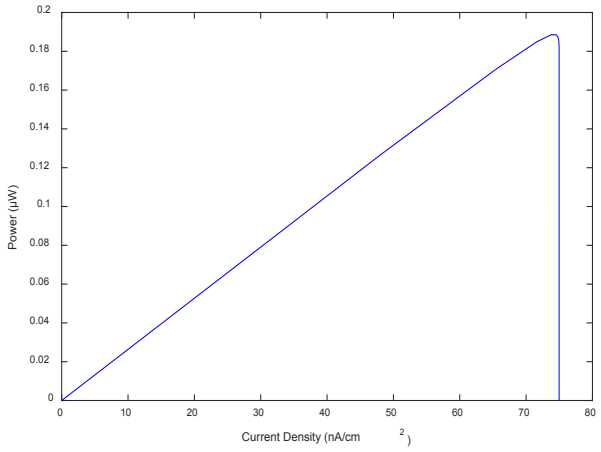

Fig. 5. Current density power (J-P) for GaN/GaN.

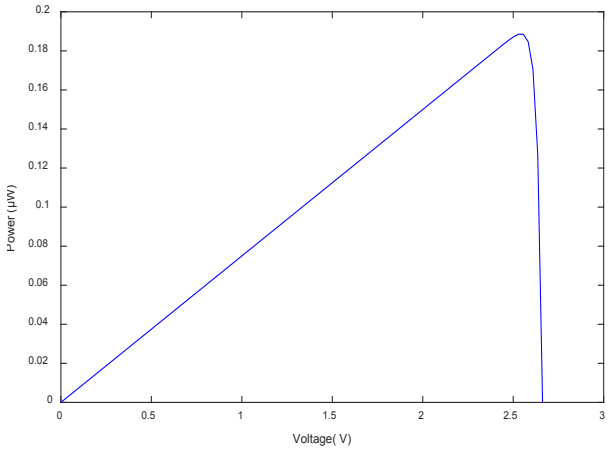

Fig. 6. Power-voltage (P-V) for GaN/GaN.

The maximum bias voltages $V_{OC} = 2.66\ V$.

The maximum current densities $J_{SC} = 74.9\ nA/cm^2$ at peak values of the power density $P_{max} = 0.18\ \mu W/cm^2$, compare with the result found in the reference [8]

$P_{max} = 17.48\ nW/mm^2$, Fill factors (FF) were determined as 94.58 % and the efficiency η= 3.14 % similar reference [8] found η= 3.3 % .

4. Conclusion

The model used allows us to obtain the spatial distributions of the electron-hole pairs generated in the materials, the energy deposition, the stopping power of each material, as well as a the efficiency of the cell that we studied.

Mainly, and in particular in order to give a more exact modeling of betavoltaic cells, has been taken to study the effect of the distribution carefully , due to particle beam, of the electron-holes pairs as being in the form of a Gaussian, in order to avoid the approximation of the existence of a zone below the surface known as ‘the death zone' (widely used by several authors to facilitate the calculations of the currents generated by solving them mathematically by analogy to cell current under photon flux). This choice is based on the fact that the best "fitting" gives a Gaussian,

which gave other solutions which differ from the solutions obtained for the junctions of the cells under photon flux.

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