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Study and modeling of a CdS /PbS betavoltaic cell by Monte Carlo simulation

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In this paper, we present simulations of the concentration of electron-hole pairs generated from each point in solid targets under Ni-63 source bombardment of a CdS/PbS-based betavoltaic cell. This model is an accurate representation of the electronic interaction has been reported. We can obtain the distribution of the electron-hole pairs generated in the CdS/PbS junction as a function of the depth by Monte Carlo simulation, this distribution allowed us to find the concentrations of excess minority carriers as a function of the thickness, which can be function and injection into the continuity equations to determine the diffusion current and then the selected petavoltage properties. The model was tested for the Ni-63 CdS/PbS structure, with energy of 17 keV.

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1. Introduction

Betavoltaic effect refers to conversion of energy from electrons generated in nuclear reactions into electricity in semiconductor p - n junctions [1]. A combination of photovoltaic development and significant reduction in electronic component power advanced betavoltaic technology in the past decade. However, studies on betavoltaic cells have been intermittent due to source availability, especially with tritium, where brief demonstrations or simulations were performed. One of the major advantages of betavoltaic cells is their performance longevity and resistance to temperature degradation. To forecast future performance, betavoltaic technology needs to be modeled to evaluate for potential implementation, especially in devices that require little to no interruption such as cardiac pacemakers and/or placed in environments where there are major temperature swings, such as extraterrestrial surfaces [2].Betavoltaics perform similarly to a solar cell where instead of photons, beta particles generate electricity. The mechanics of current generation are visualized in Figure .1. The kinetic energy of beta particles causes ionization within the semiconductor wafer by creating electron-hole pairs (EHPs). However, a large percentage of energy is lost as heat in phonon interactions and x-ray generation [3]. EHPs that do not recombine are accelerated to collectors (electrons to the n-side and holes to the p-side) due to diffusion. When a load is applied to the semiconductor wafer, electrons in the n-side travel through the load and return on the p-side, generating a current.

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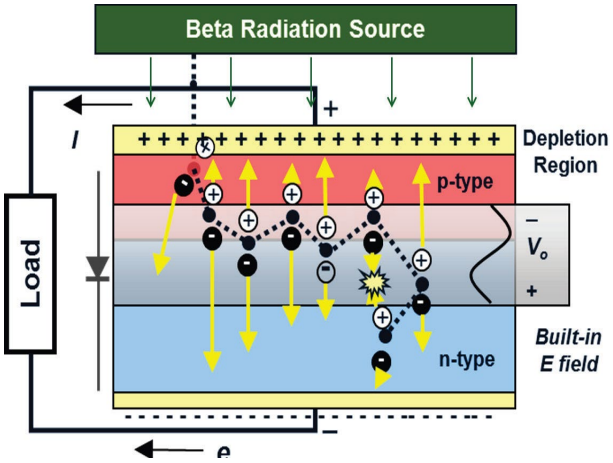


Fig. 1. Visualization of Betavoltaic Ionization [3].

Study the electron-matter interaction by separating electron-hole pairs. Various models of Monte Carlo simulation models. In some work I have relied on the Monte Carlo method to calculate the concentration of electric hole pairs generated after bombardment of a structure (semiconductor) with an electron, as found in CdS [3] using the same code and applying for PbS. The objective of this work is to rely on Monte Carlo simulations to calculate the PbS concentration of the electron-hole pairs in the material, which will allow us to calculate the current that can be generated in a P-N junction and finding the current generated without making a dead zone approximation, in order to take into account the gradient of minority carriers generated by the Ni-63 source.

2. Model

In the calculation, two consecutive elastic collisions of the incident electron are defined as one step, so that the whole motion trajectory of the electron is divided into several motion steps. Each step is composed of several inelastic collision events, and the energy loss in each step is regarded as continuous. The motion distance of each step is determined by the step length taken during the calculation and motion direction of the electron. The motion direction of the electron after each elastic collision is determined by the motion direction, as well as a series of random numbers before the collision. The energy loss of electron is calculated by the following formula [4]:

$$\frac{dE}{dS} = -7.85 \times 10^4 \frac{\rho Z}{AE} Ln\left(\frac{1.66(E+k)}{J}\right)\left(\frac{KeV}{cm}\right).$$

where J is the mean ionization potential given by[5]:

$$J = 11.5Z \ \text{(eV)} \ Z < 13$$
$$J = 9.76 + 58.5Z^{0.19} \ \text{(eV)} \ Z \geq 1$$
$$k = 0.734Z^{0.037}$$

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 [5]:

$$E_{e-h} = 2.73Eg + 0.5$$

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 by random number R (uniformly distribution between 0 and 1) 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:

$$S = -\lambda \ln(R) \quad (1)$$

where R: random number (uniformly distribution between 0 and 1)
where λ is the mean free path, can be obtain from the total scattering cross section as [5]:

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

where N_A is the Avogadro's number and σ total scattering cross section is given by:

$$\sigma = 5.21 \times 10^{21} \frac{Z^2 4\pi\lambda_c\left(1 - e^{-\beta\sqrt{E}}\right)}{E^2\left(\delta(\delta+1)\right)} \left(\frac{E + m_0C^2}{E + 2 \times m_0C^2}\right)^2$$

where δ is a screening parameter given by[5]:

$$\delta = (3.4 \times 10 - 3)\left(10^{0.67}/_{E}\right)$$

λ_C and β are constants for a given element[6],

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

The angle α for particular scattering event can be obtained from the probability by the relationship [7]:

$$\cos \propto = 1 - \frac{2\delta R}{1 + \delta - R}$$

The azimuthal angle θ is given by [8]:
$\theta = (1 - 2R_1)_1$ 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 $\theta > \pi/2$ or $\theta < -\pi/2$ the electron leaves the matter and will be supposed to be backscattered electron, only angles between $-\pi/2$ and $\pi/2$ enter the matter.

3. Results and discussion

Monte Carlo methods are ubiquitous in the theory of condensed matter, they make it possible to obtain "exact" measurements in direct comparison with the stopping range found by Kanaya and Okayama to validate the results. Concerning our model, the calculations show that the trajectory of 50 electrons in a sample of PbS. To calculate the stopping range proposed by our model we take the average penetration of 50 electrons:

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

where n is the number of incident electron in our case equal 50.r_{max} is the maximum distance of the electron travels in the matter before losing all of its energy and stopping, 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. The stopping range finding by Kanaya and Okayama relationship given by [9]:

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

This relationship validated for energies $E0$ (incident energy of the electron) between 0-1000 KeV.

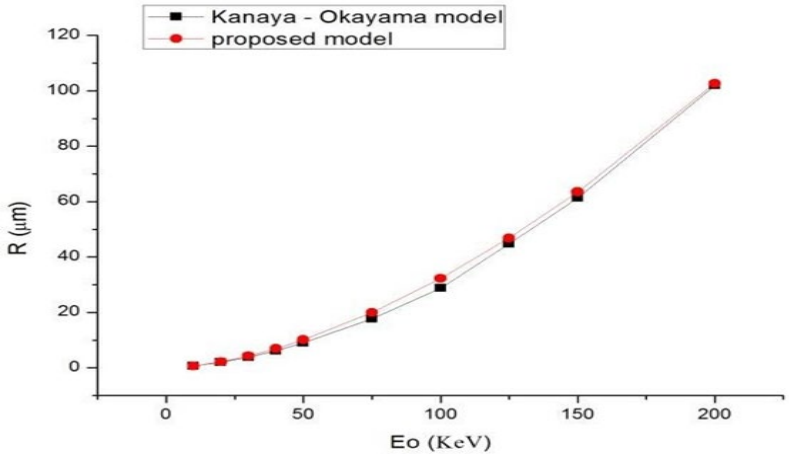
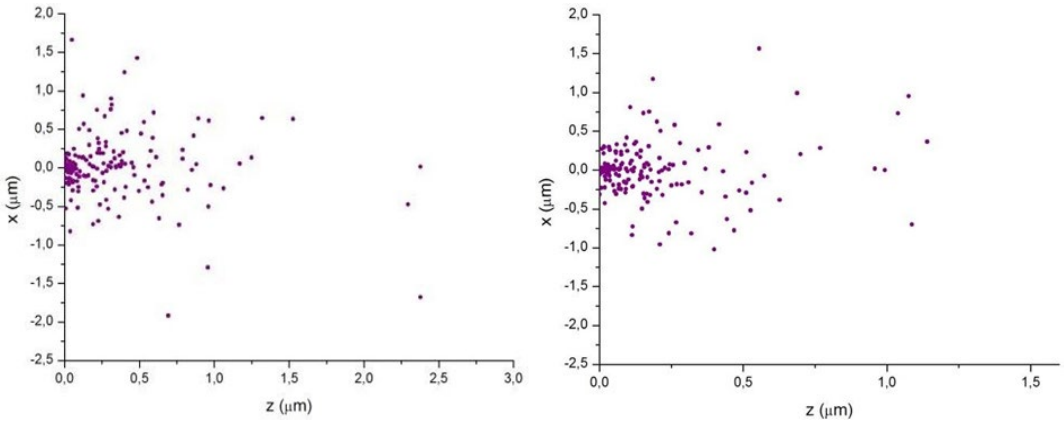


Fig. 2. Stopping range of electrons in CdS as function of acceleration energy.

We calculate the concentration of the electron-hole pairs generated after a bombardment of a CdS semiconductor with a beam of electron with energy $E0 = 17\ KeV$ (Fig .3.). this electron undergoes elastic and inelastic collisions by creating pairs of electrons holes and losing its energy between each two collisions until the PbS semiconductor, where the parameter changes and the the bomardement energy for PbS $E0 = 16.58\ KeV$.



(a) *(b)*

Fig.3. The distribution of electron-hole pairs generated as a function of depth in. a.CdS. b. PbS for an acceleration energy 17 KeV.

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.4.) for energies 17 KeV.

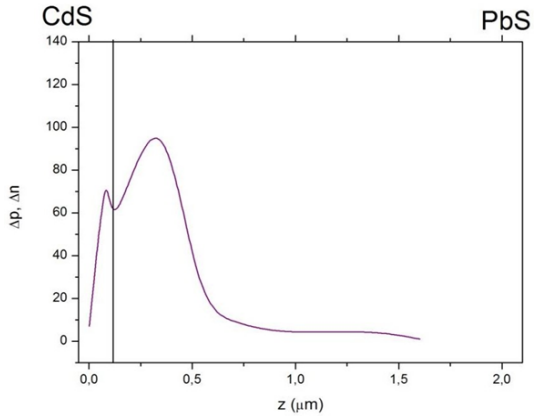


Fig. 4. The distribution of the concentration of electron-hole pairs generated by inelastic collisions of the incident electron in CdS/PbS.

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)

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

where: a,b,c are constants for each cells present in (Table 1):

Table 1. Fit function G_{ph} constants for CdS and PbS cells.

Incident energy (KeV)	CdS(n)		
	A	B	C
71	91.884	0.0020098	0.0013206
Incident energy (KeV)	PbS(p)		
	A	b	c
71	152.07	0.0027868	0.0016445

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 CdS/ PbS based betavoltaic cell, the parameter for CdS/ PbS cells used in our simulation are grouped in the following table:

Table 2. The parameters of CdS/ PbS.

	$E_g\,(eV)$	$N_d\ cm^{-3}$	$N_a cm^{-3}$	n type thickness (cm)	p type thickness (cm)
$CdS_{(n)}$	2.42	10^{19}	--	0.1 μm	--
$PbS_{(p)}$	0.41	--	10^{14}	--	2 μm

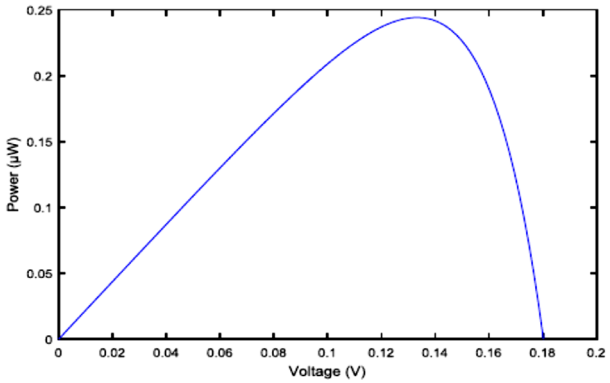


Fig. 5. Current Density voltage for CdS/PbS.

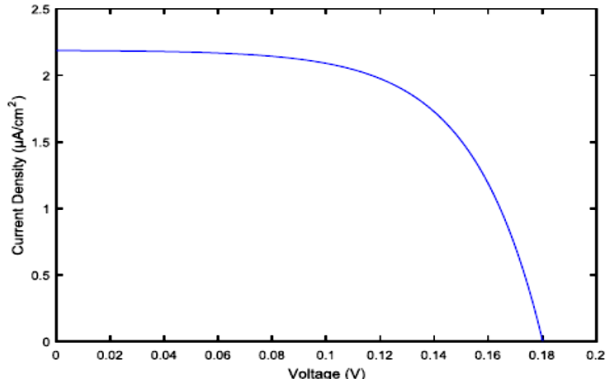


Fig. 6. Current density power (J-P) for CdS/PbS.

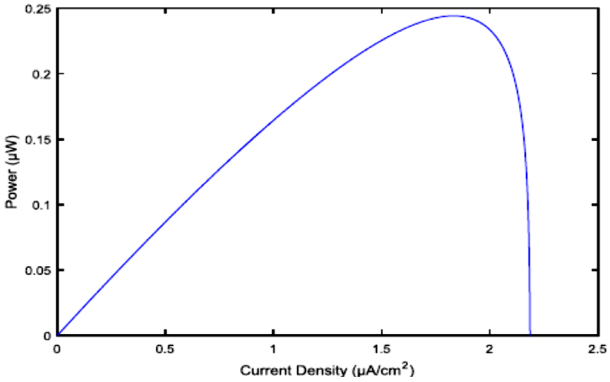


Fig. 7. Power-voltage (P-V) for CdS/PbS.

The absolute current density versus the bias voltage variation as shown in (fig .5.), Maximum bias voltages V_{0C} = 0.18V, and maximum current densities J_{SC} =2.18 $\mu A/cm2$ at peak

values of the power density P_{max} = 0.24 μW/$cm2$, Fill factors (FF) were determined as 61.9 % and the efficiency η= 4.08 %.

4. Conclusions

Monte Carlo method is a statistical technique for obtaining numerical solutions to physical or mathematical problems that are analytically impractical, if not impossible, to solve. For charged particle transport problems, it presents many advantages over deterministic methods since such problems require a realistic description of the problem geometry, as well as detailed tracking of every source particle. Thus, MC can be considered as a powerful alternative to the well-known Bethe-Bloche equation where an equation with various corrections is used to obtain stopping power and ranges of electrons, positrons, protons, alphas, etc. This study presents how a stochastic method such as MC can be utilized 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.

The aim of this work being to give a more precise modeling of betavoltaic cells, we tried to carefully study the effect of the distribution, due to the particle beam, of the electron-hole pairs as being in Gaussian form, in order to Avoid approximating the existence of an underground region called the 'death zone'. This choice is based on the fact that a better "fit" gives a Gaussian image, which gave other solutions which differed from the solutions obtained for cell junctions under photon flux. Our results are compared with those of the literature, as well as other theoretical results and they are in good agreement. This comparison made it possible to deduce values for the physical parameters on the one hand, and to make a correspondence between the physical parameters introduced in different models on the other hand, and the coherent reconciliation between different models.

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