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# Modelling and simulation of PN junction CdS/CdTe for betavoltaic cell

A. Talhi[a,*], B. Azeddine[b,c], Z. Tiouti[c], M. Rajczyk[d]
[a]*Laboratory of Environmental and Energetic Systems , University Centre Ali Kafi Tindouf, Algeria*
[b]*Laboratory for the Development of Renewable Energies and their Applications in Saharian Areas; University Tahri Mohammed Bechar, Algeria*
[c]*Laboratory of Physics and Semiconductors Devices, University Tahri Mohammed Bechar, Algeria*
[d]*Politechnika Częstochowska, University of Technology, Poland*

The method for producing power by integrating a beta source to semiconductors junction's devices is called as betavoltaic energy conversion. [1]. In this study by using Monte Carlo (MC) method to simulate the distribution of electron- hole pairs (EHP) generated at each point in the cell under bombardment of $^{63}$Ni source for betavoltaic cell then the result of that Monte Carlo simulation will be used in the modelling and simulation of a betavoltaic cell CdS/CdTe heterojunction and their characteristics.

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*Keywords:* Monte Carlo method, Interaction, Betavoltaic cell, Generation EHP, CdS, CdTe, Heterojunction

## 1. Introduction

Utilizing semiconductors, betavoltaic or alphavoltaic batteries draw power from radioisotope sources that emit beta or alpha radiations. In the semiconductor, the radioisotope's beta particles kinetic energy is transformed into electrical power [2]. They have the advantages of high energy density, long service life, strong anti-interference ability, small size, light weight, easy miniaturization and integration, thus it has become a research in the field of micro energy. Betavoltaic batteries operate similarly to photovoltaic cells in terms of their core principles. By impact ionizing the electrons, the beta particles (electrons) released by the decay of radioactive isotopes strike semiconductor device like p-n, p-i-n, or Schottky junction to create electron-hole pairs in the surrounding matter. The electron-hole pairs are then separated and gathered to produce electricity [3,4]. In this paper we are interesting in interaction between electron and matter to create pairs electron-hole by using Monte Carlo simulation model. This method using to calculate concentration of electron-hole pairs in matter generated after bombardement of semiconductor with electron beam then the results will be injected as function into continuity equations to determinate a generated current. The model of betavoltaic cell proposed to study is CdS/CdTe for average energy 17 KeV.

## 2. Physical approach simulation

The electron trajectory simulation treat of electron elastic and inelastic scattering, the trajectory is random, our simulation is based on. The inelastic interaction effect witch result in the loss of energy after each shock of this type of interaction and the random number draw for found, electron trajectory, collision position, secondary electron, the concentration of electron-hole pairs generated, and the distribution of the concentration of electron-hole pairs generated. The present

*Corresponding author: karim.talhi@gmail.com
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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 in straight line between random scattering events (elastic collision or inelastic).

The step ***S*** length is derived from [5,6]:

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

$\lambda$ : mean free path, it's obtain by the total scattering cross section [4, 5, 6]

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

$A$ is atomic weight ; $\rho$ is the density of the semiconductor and $N_A$ is Avogadro's constant.
The total scattering cross section $\sigma$ is [6]:

$$\sigma = 5.21\times10^{-21}\frac{Z^2 4\pi\lambda_c\left(1-e^{-\beta\sqrt{E}}\right)}{E^2\delta(\delta+1)}\left(\frac{E+m_0c^2}{E+2m_0c^2}\right) \tag{3}$$

$Z$ is the atomic number of the scattering atom; $E$ is the energy of electron in $KeV$ .
$\delta$ is a screening parameter given by [6, 7]:

$$\delta = \left(3.4\times10^{-3}\right)\frac{Z^{2/3}}{E} \tag{4}$$

$\beta$ ; $\lambda_c$ : constants where[7] : $\beta = \frac{26.42}{Z^{1.24}}$ and $\lambda_c = 1.162 + 1.28\times10^{-2}Z$

The angle $\alpha$ for particular scattering, it obtained from the probability [5]:

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

We define the azimuthally angle by [4]:

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

Where $R_1$ represents random number $(0 < R_1 < 1)$ and $\theta$ is angle $(-\pi < \theta < \pi)$.We assume that the incident electron travels parallel to the surface normal 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. The electron lost energy between two collisions is defined by [7]:

$$\frac{dE}{dS}(KeV/cm) = -7.85\times10^4\frac{\rho Z}{AE}\ln\left(\frac{1.166(E+kJ)}{J}\right) \tag{7}$$

$k = 0.734 \times Z^{0.037}$ and $J$ is the ionization potential given by [5,7]:

$$\begin{cases} J(eV) = 11.5 \times Z & Z < 13 \\ J(eV) = 9.76 + 58.5 \times Z^{0.19} & Z \geq 13 \end{cases} \quad (8)$$

After inelastic collision the electron lost also energy $E_{e \to h}$ to generate one pair electron-hole. The electron –hole pairs creation energy can be taken [8,6]:

$$E_{e \to h}(eV) = 2.73 \times E_g + 0.5 \quad (9)$$

## 3. Results of simulation

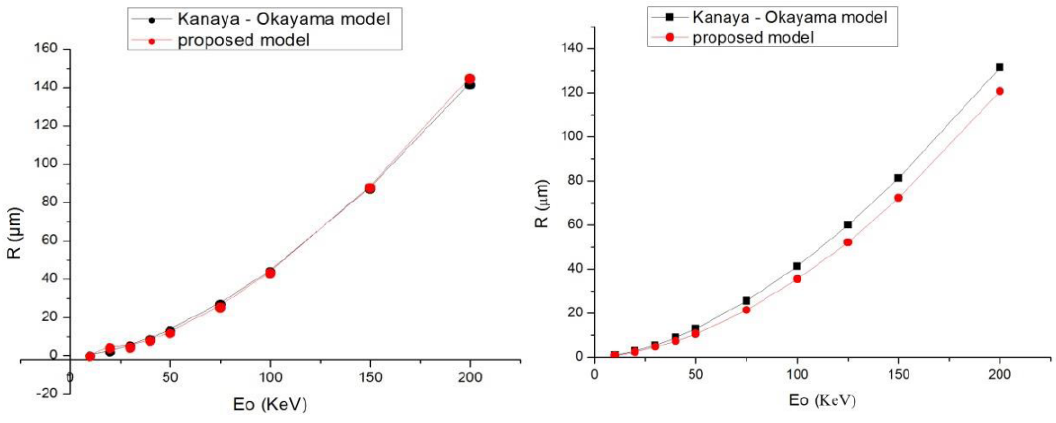
### 3.1. Penetration depth

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's collisions with atoms and the energy losses in inelastic collisions and between two collisions. The stopping range of the CdS was done [4] and we calculate using M.C code for CdTe semiconductor by our model and we compare with the stopping range funded by Kanaya and Okayama model, it will validate our results of proposed method. The stopping range proposed in this simulation with $200$ electrons for average of penetration is [9, 4]:

$$R = \frac{\sum_{i=1}^{n} r_{\max}}{n} \quad (10)$$

$n$ is number of incident electron in our study is 200 ; $r_{\max}$ is maximum distance electron penetration depth in matter for every electron. The Kayana and Okayama model is defined as [9]:

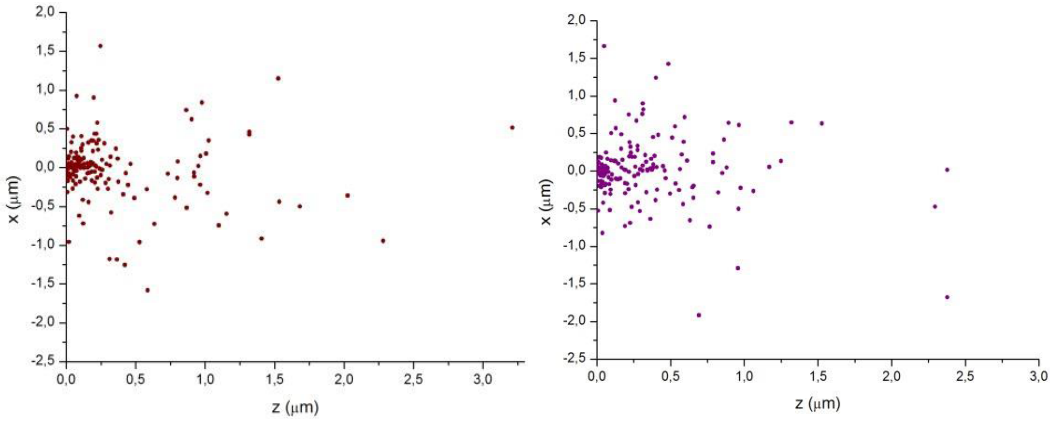
$$R = \frac{2.76 \times 10^{-11}}{\rho} \times \frac{A \times (E_0)^{\frac{5}{3}}}{Z^{\frac{8}{9}}} \times \frac{\left(1 + 0.978 \times 10^{-6} E_0\right)^{\frac{5}{3}}}{\left(1 + 0.978 \times 10^{-6} E_0\right)^{\frac{4}{3}}} \quad (11)$$




*CdS [4]* *CdTe*

*Fig. 1. Stopping range of electrons for CdS and CdTe materials as function of acceleration energy.*

Fig. 1 represents the stopping range calculated by our model based on Monte Carlo method for CdS [4] and CdTe. A comparison was made between the penetration depths found by our models and that of Kanaya and Okayama. Our model clearly shows that the depth of penetration of electrons incidents grows as a function of the accelerating energy of the incident beam. The method proposed matches the Kanaya and Okayama model.




*CdS[4]* *CdTe*

*Fig. 2. The spatial distribution of electron-hole pairs generated as a function of depth in CdS [4] and CdTe For average energy 17 KeV.*

The Fig. 2 present the spatial distribution of electron-hole pairs generated during inelastic collisions after a bombardment of one electron, taking the average of several tests, if $\left(E > E_{e \to h}\right)$ an electron-hole pair forms, we calculate the energy variation.

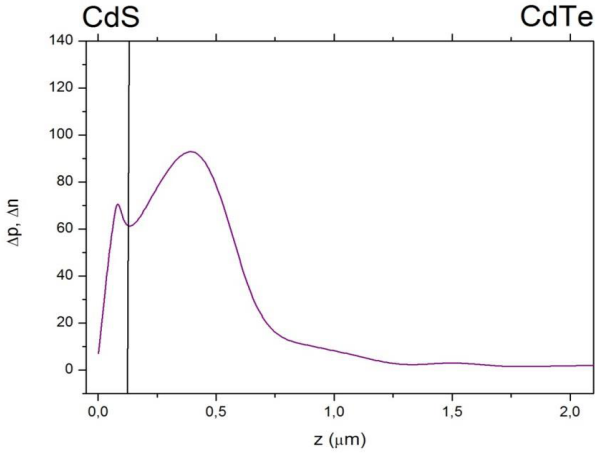



*Fig. 3. The distribution of the concentration of electron-hole pairs generated by inelastic collisions of the incident electron with CdS/CdTe.*

The sample is partitioned into a number of zones. Quantities of electron-hole pairs are produced at each zone, and the profile of their generation is dependent on the thickness of the zone $z$. The energy incident for CdS [4] is $E_0 = 17\,KeV$ after losing some energy in depth $0.1\mu m$, will enter the CdTe semiconductor, where the parameter changes and the bombardment energy for CdTe will be $E_0 = 16.08\,KeV$ after calculation (Fig.03).The variation of the minority charge

carriers $\Delta n(x)$ in the p-type semiconductor and $\Delta p(x)$ in the n-type semiconductor is calculated as a function of the depth.

### 3.2. Characterisation of betavoltaic CdS/CdTe Cell:

The distribution of the concentration EHP generated by the incident electron in the structure, we define the $G_{ph}$ as a function of concentration EHP generated depending the thickness $x$ :

$$G_{ph} = a\, e^{-\left(\frac{x-b}{c}\right)^2} \quad (11)$$

*Table 1. Full function $G_{ph}$ constants for CdS/CdTe cell [10].*

| **Incident energy KeV** | **CdS (n)** | | |
|---|---|---|---|
| 17 KeV | a | b | c |
| | 91.884 | 0.0020098 | 0.001325 |
| **Incident energy KeV** | **CdTe (p)** | | |
| 16.08 KeV | a | b | c |
| | 151.83 | 0.0033572 | 0.00209 |

In order to determine the concentrations of the minority charge carriers, we must solve the continuity equations while taking the $G_{ph}$ function into consideration in order to estimate the current flowing through the junction. The parameters of simulation used to CdS /CdTe based betavoltaic are assembled in table 2.

*Table2.The parameters of CdS /CdTe cell.*

| | Gap eV | $N_d\ cm^{-3}$ | $N_a\ cm^{-3}$ | Thickness |
|---|---|---|---|---|
| CdS (n-type) | 2.42 | $10^{19}$ | -- | $0.1\,\mu m$ |
| CdTe ( p-type) | 1.44 | -- | $10^{16}$ | $2\,\mu m$ |

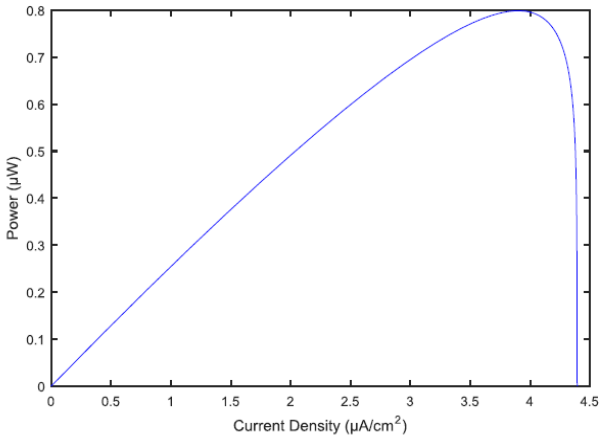



*Fig. 4. Current density voltage (J-V) for CdS/CdTe.*

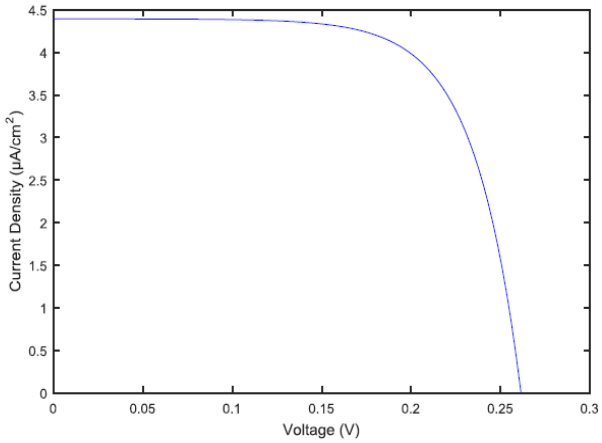



*Fig. 5. Current density power (J-P) for CdS/CdTe.*

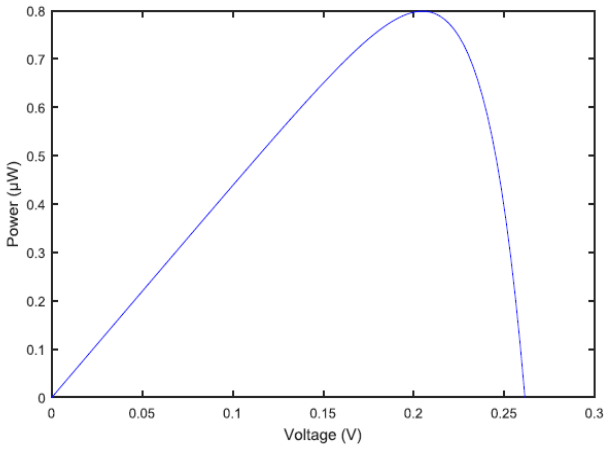



*Fig. 6. Power voltage (P-V) for CdS/CdTe.*

Parameters of this cell are:

| $V_{co}$ | $J_{sc}$ | $P_{\max}$ | $FF$ | $\eta\%$ |
|---|---|---|---|---|
| $0.26V$ | $4.39\,\mu A/cm^2$ | $0.79\,\mu W/cm^2$ | 69.62% | 13.34% |

## 4. Conclusion

In this work, we were able to provide a realistic depiction of the effects of a particle beam on matter due to the application of the Monte Carlo method, taking into account the nature of the sources that can be used radio potentially and not harmful as radioactive sources. The model we employed gives us the ability to determine the spatial distributions of the electron-hole pairs produced in the materials. Distribution of the electron-pair holes carefully due to particle beam has been carefully studied in order to avoid approximating the existence of a zone below the surface known as "the death zone," and in particular to give a more accurate modelling of betavoltaic cells. This decision is supported by the Gaussian solution provided by the best fitting which provided other solutions that are distinct from those found for the junction of the cell subjected to photon flux. The particle source was $^{63}$Ni, which was used including the junction n-CdS/p-CdTe. The CdS/CdTe junction showed good efficiency, which can be explained by the fact that the incident particle's energy is deposited to form the most EPHs in inelastic shocks, and the least amount of

energy is deposited in the electronic cloud between two collisions(elastic and/or inelastic). This is because CdS and CdTe have a lower density than other materials, which results in more energy being deposited in EHPs in inelastic shocks.

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