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THE CONCENTRATION OF ELECTRON-HOLE PAIRS GENERATED BY THE INTERACTION OF ELECTRON WITH MATTER, CASE OF CdS USING MONTE CARLO SIMULATION

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In this study, we use a Monte Carlo Calculation code to simulate the stopping range and the concentration of electron-hole pairs generated of each point in the solid targets under a bombardment, those electrons and holes generating a low electrical power source for many specialized applications.
The model has been tested for CdS structure, under a bombardment of one electron with energy 50 - 150 KeV.

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1. Introduction

Numerous fields require a power sources with low power and long lifetime such as biomedical, military applications, space equipment, sensors in remote location and implantable medical devices..etc[1]. Many approaches have been proposed to develop this power source, such as harvesting ambient heat, vibration energy, solar energy….etc[2].

The semiconductor used in this study, cadmium sulphide (CdS) thin films group II-VI have high transparency, wide and direct band gap transition, high electron affinity and n-type conductivity, CdS are considered as a promising semiconductor material for the development of many interesting and wide applications in the field of solid-state solar cells, light emitting diodes[3], photoconductor, photocatalysts, electrochemical cell, gas sensor, and photosensor etc..[4].

In this work we calculate the concentration of the electro-hole pairs generated after a bombardment of a CdS semiconductor with an electron of energy 50 – 150 KeV.

The incident electron will flow from arrival at the surface until the end of its path inside a semiconductor, this electron undergoes elastic and inelastic collisions by creating pairs of electrons holes and losing its energy between each two shocks.

2. Model

After a bombardment of the target with one electron, we propose a code to calculate the concentration of electron-hole pairs generated by inelastic collisions, during the collision of the incident electron with the atoms of the target, while taking into account elastic collisions.

After each collision the electron lost energy, the rate of loss energy used in this simulation given by [5]:

$$\frac{dE}{dS} = -7.85 \times 10^4 \frac{\rho Z}{AE} \ln\left(\frac{1.166(E+kJ)}{J}\right) \text{(KeV/cm)} \quad (1)$$

where Z is the atomic number of the scattering atom, E is the energy of electron in KeV, A is atomic weight, ρ: is the density of the semiconductor.

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

$$J = 11.5Z \ \text{(eV)} \qquad Z < 13$$
$$J = 9.76 + 58.5Z^{0.19} \ \text{(eV)} \quad Z \geq 13$$

Parameters for the relation (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 [6]:

$$E_{e-h} \approx 3E_g \tag{2}$$

where E_g is band gap energy.

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. The step length S is derived from[7]:

$$S = -\lambda \ln(R) \tag{3}$$

where λ is the mean free path, can be obtain from the total scattering cross section as[7]:

$$\lambda_m = \frac{A}{N_A \rho \sigma} \tag{4}$$

where N_A is the Avogadro's number, and σ is the total scattering cross section is given by[5]:

$$\sigma = 5.21 \times 10^{-21} \frac{Z^2}{E^2} \frac{4\pi\lambda_c\left(1 - e^{-\beta\sqrt{E}}\right)}{\delta(\delta+1)} \left(\frac{E + m_0 c^2}{E + 2 \times m_0 c^2}\right)^2 \tag{5}$$

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

$$\delta = (3.4 \times 10^{-3}) \frac{10^{0.67}}{E} \tag{6}$$

λ_c and β are constants for a given element[5],

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

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

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

$$\cos\alpha = 1 - \frac{2\delta R}{1 + \delta - R} \tag{7}$$

The azimuthal angle θ is given by:

$$\theta = (1 - 2R_1)\pi \tag{8}$$

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.

The elastic or inelastic scattering depends on α

Table 1. Parameter for CdS used in our model.

Parameter	CdS
Energy band gap E_g(eV)	2.42
Density ρ(g/cm^3)	4.826
Atomic number $Z = Z_{Cd} + Z_S$	64
Atomic weight A (g/mol)	144.477

3. Results and discussion

We calculate the stopping range of the CdS semiconductor by our model 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 50 electrons:

$$R = \frac{\sum_{i=1}^{n} r_{max}}{n} \tag{9}$$

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[8]:

$$R = \frac{2.76\times10^{-11}}{\rho}\frac{A\times(E_0)^{5/3}}{Z^{8/9}}\frac{(1+0.978\times10^{-6}E_0)^{5/3}}{(1+1.957\times10^{-6}E_0)^{4/3}} \tag{10}$$

This relationship validated for energies E_0 (incident energy of the electron) between 0-1000 KeV

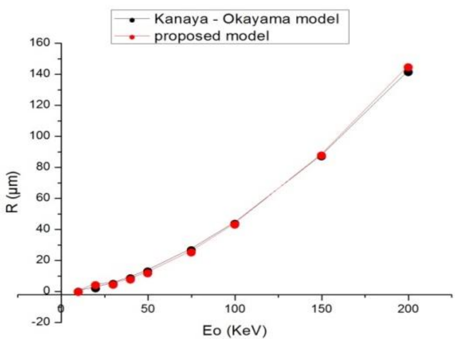

Fig. 1. Stopping range of electrons in CdS as function of acceleration energy.

The Fig. 2 shows the distribution of electron-hole pairs generated during collisions, after a bombardment of one electron, taking the average of several tests.

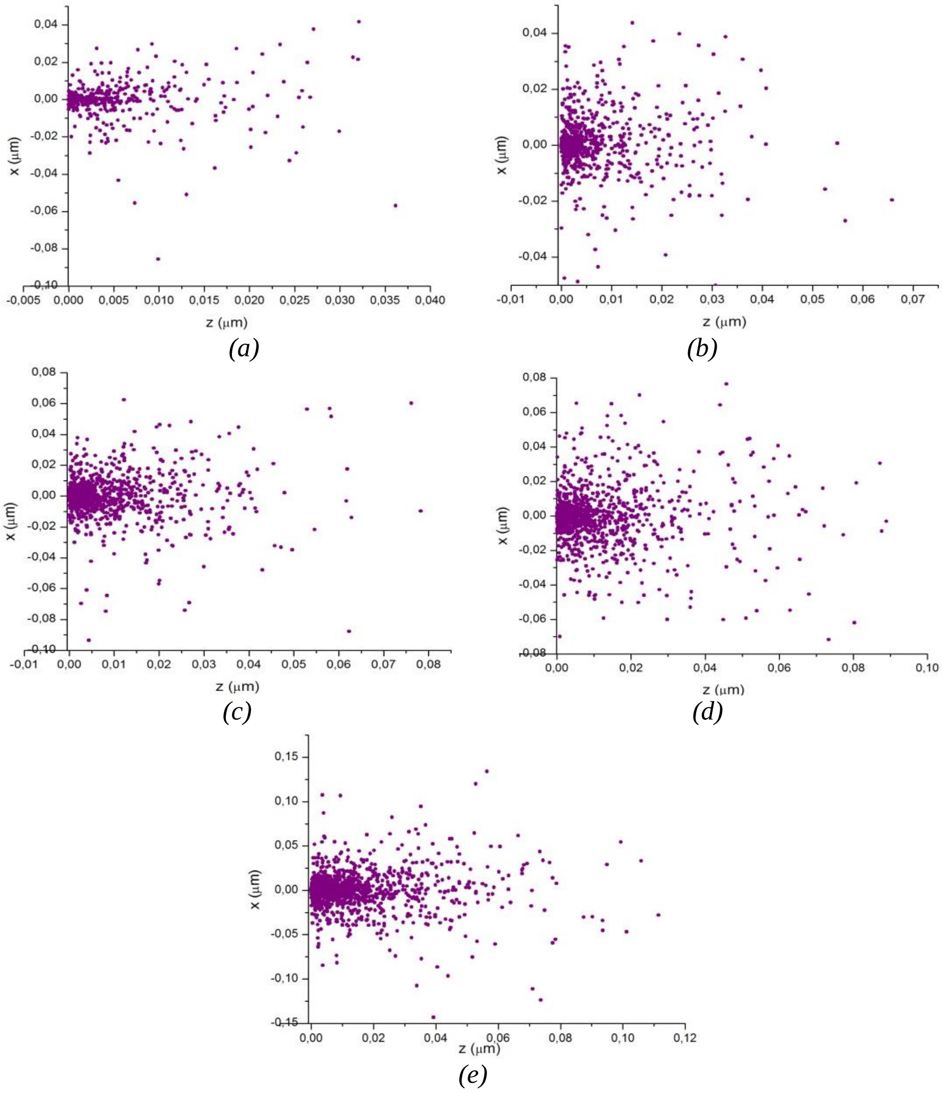

Fig. 2. The distribution of electron-hole pairs generated as a function of depth in CdS structure for an acceleration energy a. 50 KeV, b. 75 KeV, c. 100KeV, d.125KeV, e.150KeV.

The Fig. 3 shows the distribution of the concentration of electron-hole pairs generated for different energies of incident electron.

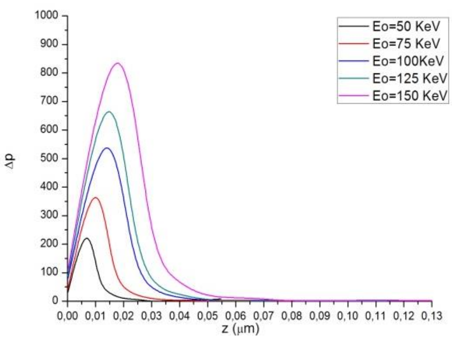

Fig. 3. The distribution of the concentration of electron-hole pairs generated by inelastic collisions of the incident electron with CdS structure for an acceleration energy 50-150 KeV.

4. Conclusion

This study presented a Monte Carlo model simulation of interaction of one electron with a matter in our case with a semiconductor CdS; the result, from this simulation we can obtain the distribution of electron-hole pairs generated in CdS as a function of the depth and energies.

This method can be used for all interactions of particles with matter, such as electrons (beta radiation), alpha radiation, protons neutrons, using the same calculation taking into account the Bethe equations for heavy or light particles, charged or not.

This result, which is the profile of the distribution of electron-hole pairs in matter, is very important to calculate the current that can be generated in a p-n junction or Schottky junction (metal/SC) solar cells, the distribution of electron-hole pairs in matter has 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 which can take place, as well this profile can give the conduction current generated in depletion zone (ZCE) separately.

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