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Effect of Manganese concentration in the $Cd_{1-x}Mn_xTe/CdTe$ Tandem structure on photovoltaic energy conversion

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Abstract

The photovoltaic electricity is obtained by direct conversion of sunlight into electricity by solar cells. The objective of this work is the study and simulation of a Tandem photovoltaic structure based on $Cd_{1-x}Mn_xTe$ as top material cell. This paper describes the optimization of energy efficiency for $Cd_{1-x}Mn_xTe$ thin films deposited by epitaxy on CdTe substrat. We present the impact of the manganese concentration in $Cd_{1-x}Mn_xTe$ thin films on solar cells performances. Our study includes simulation results to show the conversion efficiency and main performances factors as function of the manganese concentration.

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1. Introduction

Specific properties of CdTe made it as a perfect material for some applications, e.g solar cells, sensors, electro-optic modulators of high efficiency and photorefractive devices. This material may have both types of conductivities n and p which made diode technology [1, 2] and the field-effect transistors [3]. Semi-conductors made by CdTe as CdMnTe, have extremely exciting properties that until now not fully exploited [4]. CdTe is a ternary alloy consisting of CdHgTe, which is one of the main industrials for infrared detection. CdZnTe is used as substrate for the deposition epitaxy HgCdTe layers and as a nuclear detector, which suggest a great potential application mainly for medical purposes. Physic of semi-conductors development is around the porous silicon and semi-conductors structures II-VI and III-V. Various quantum hetero-structures more or less complex (well , wires, self-organized quantum dots, laser structures , microcavities) are developed with II-VIT ellurides family (CdTe , ZnTe , MnTe , MgTe) and Nitrides with more large gap (GaN, InN, AlN). This work focuses on the main electrical and optical properties of CdMnTe alloy (with the incorporation of manganese). We will study the influence of the manganese incorporation on the characteristics of CdMnTe/CdTe structure: the band gap energy, transition energy, the strain, the reflection coefficient, the reflective index and the optical power emitted. This paper presents the structure and principle of cell photovoltaic's operation. We then give the electrical parameters of a cell-based structure of our $Cd_{1-x}Mn_xTe/CdTe$. We can identify several electronic parameters of an alloy, by linear interpolation of binary parameters parents who compose it, from the relationship of "Vegard's law":

$$P(A_{1-x-y}B_xC_yD)=(1-x-y)PAD+ xPBD+ yPCD \quad (1)$$

2. Theoretical approach

2.1. Lattice parameter

The lattice parameter is defined as the distance between two consecutive lattices. The table 1 [5,6] gives the lattice parameters in the zinc-blend structure of our material .

Table 1. Lattice parameter of used binary materials

compound	a(A°)
CdTe	6.481
MnTe	6.337

The lattice parameter of Cd_{1-x}Mn_x is calculated using Vegard’s law

$$a_{Cd(1-x)Mn(x)Te} = (1-x)a_{CdTe} + x a_{MnTe} \tag{2}$$

2.2strains and relaxation

When the epitaxial growth of a material on a substrate of different lattice parameter, a compressive or a biaxial expansion strain occurs on the layer epitaxed, which is accompanied by an elastic energy accumulation. Beyond a critical thickness, the elastic energy stored is sufficient to generate structural defects which partially relax the strain in the crystal. The material then tends to resume its lattice parameter, and dislocations appear at the interface (plastic relaxation).The critical thickness depends directly on the difference of lattice parameter between substrate and layer [7]. Elastic deformation of network appears perpendicularly to the plan of growth (figure 1).

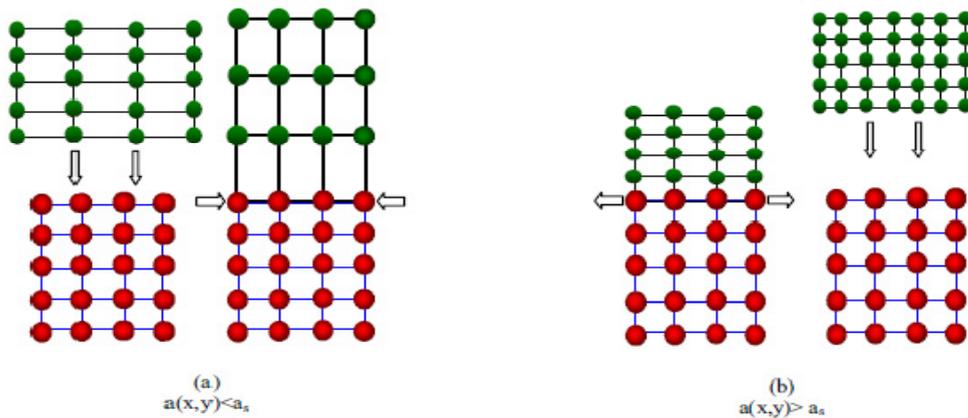


Figure 1.epitaxy of mismatch lattice parameter layer (a) in compression and (b) in strain on a substrate that lattice parameter is a₀. [8,9]

In the case of a standard rigid substrate very thick, the constraints are substantially borne by the growing layer. Its strain rate is a function of the lattice mismatch with the substrate. This disagreement is defined by [8].

$$\epsilon = \frac{\Delta a}{a} = \frac{a_s - a_e}{a_s} \tag{3}$$

Where a_s and a_e are respectively the lattice parameters of substrate and the natural layer epitaxed. If ε is positive, the layer is in “tension” and if it is negative the layer is in “compression”. The alloy Cd_{1-x}Mn_xTe has a

direct gap which varies almost linearly with Mn's composition [10]. The biaxial strain can be decomposed into a hydrostatic term and a shear component. The first changes the band gap, whereas the shears lift the degeneracy of the valence band between heavy and light holes [7]. When the solar irradiation enters a semiconductor, a part of this radiation is reflected, another is absorbed and the last passes through the layer of material without being absorbed. The optical properties of a solid are in dependence of the conventional band diagram in reciprocal space k [11]. The electric structure of CdTe shows a direct gap semiconductor, whose band structure allows important vertical radiative transitions between valence band and conduction band. This property is the main purpose of his application in optoelectronic's field. CdTe has a wide band gap of about 1,51 eV at room temperature (300 °K), which gives a threshold optical absorption in infrared field, particularly infrared sensing and as a substrate for epitaxy of CdMnTe layers. During the path of light in the solar cell active layer, a photon can be absorbed by this layer to produce an electron-hole pair [12]. The absorption coefficient α for photon energy greater than the gap energy is given by the following formula:

$$\alpha = \alpha_0 \frac{\sqrt{E-E_g}}{E} \quad (4)$$

where $\alpha_0 = 5 \cdot 10^5 \text{ cm}^{-1}$

The variation of refractive index is calculated using empirical Herve and Vandamme's formula, which is a function of band gap energy:

$$n = \sqrt{1 + \left(\frac{A}{E_g + B}\right)^2} \quad (5)$$

where A and B having the values 6.13 and 3.4eV, respectively. In fact, the semiconductor refractive index is fundamental physical parameters which characterize optical and electrical property [13].

2.2.1 Reflection

The reflection law says that for specular reflection, the angle at which the wave is incident on surface equals the angle at which it is reflected. The reflection coefficient is defined by the following formula:

$$R = \left(\frac{1-n}{1+n}\right)^2 \quad (6)$$

Where n is the layer reflective index.

3. Solar cell parameters :

The solar cell is just another photodiode that operates without external bias and supply its photocurrent in a load. Definition of cell's parameters is performed from the current voltage characteristic. We can observe that, in darkness, the solar cell has diode behavior. Under illumination, the various parameters characterizing the photovoltaic cell can be determined in according to the shape of the curve in the fourth quadrant: There is [14]:

$$I = I_{ph} - I_s (e^{V/KT} - 1) \quad (7)$$

The first term of the expression is the photo-current; the second is a direct current resulting from the bias of the diode in the forward sense by the voltage V which appears across the load resistor. The photocurrent is a function of the absorption coefficient, the incident flow and the width of the depletion region. To calculate photocurrent we plot the variation of the number of photons absorbed with respect of Manganese concentration.

3.1 Short-circuit current I_{CC} .

This is the current supplied by the cell when the voltage across its terminal is zero. It increases with the intensity of illumination of the cell and depends on the illuminated surface, the radiation wavelength, the carrier mobility and temperature [15]. The short circuit current is the obtained current when the cell terminals are short circuited ($V=0$). It decreases with the manganese concentration.

3.2 Open circuit voltage , V_{oc}

The open circuit voltage represents the voltage across the cell under illumination without charging circuit. It depends on the type of solar cell (pn junction, Schottky junction), materials of active layer and nature of contacts. It also depends on the cell illumination. That is the maximum potential that the cell can provide when the current is zero. It is given by :

$$V_{OC} = \frac{E_g}{q} - \frac{KT}{q} \ln\left(\frac{I_0}{I_{cc}}\right) \quad (8)$$

3.3 Power output :

The power supplied by the battery is given by the product $V I$.

$$P = VI = V (I_{ph} - I_S(e^{eV/KT} - 1)) \quad (9)$$

This power is maximum at the point P_m , defined by $dp/dv = 0$,

$$\text{i.e } I_{ph} - I_S(e^{eV/KT} - 1) - I_S \frac{eV}{KT} e^{eV/KT} = 0 \quad (10)$$

The voltage V_m and I_m at the point P_m are given by

$$\left(1 + \frac{eV}{KT}\right) e^{\frac{eV_m}{KT}} = 1 + \frac{I_{ph}}{I_S} \quad (11)$$

$$I_m = I_S \frac{eV_m}{KT} e^{\frac{eV_m}{KT}} \quad (12)$$

The power output is then given by the product $V_m I_m$ as

$$P_m = V_m I_m = FF V_{oc} I_{cc} \quad (13)$$

FF is the form factor.

3.4 Form factor

The parameter FF is the fill factor or form factor; it measures the rectangular character of the curve I-V. This is a ratio that reflects the quality of its I(V) curve form. It is defined by the following equation [12].

$$FF = \frac{V_m I_m}{V_{oc} I_{cc}} \quad (14)$$

3.5 Efficiency

The conversion efficiency for solar cells refers to the ability of the cell to cover the photon energy [16]. The efficiency of the solar cell is given by the ratio of the maximum power available to the incident radiation power. It represents the external energetic efficiency of power conversion.

$$\eta = \frac{P_m}{P_0} = FF \frac{V_{oc} I_{cc}}{P_0} \quad (15)$$

The expression shows that the solar cell performance is resulting directly from the three parameters values I_{cc} , V_{oc} and FF. The parameters are from part a function of the specific properties of the material, such that gap, absorption and reflection coefficients, diffusion length of the carrier or surface recombination velocity; and from other part technological parameters such the depth of junction, width of the space charge zone and the presence of parasitic resistances.

4. Results and discussion

The figure 2 represents the variation of the lattice mismatch as a function of the x% Manganese concentration. We see a small mismatch between the epitaxial layer $Cd_{1-x}Mn_xTe$ and CdTe substrate. For $x=0\%$ we have a lattice mismatch $\epsilon=0$ and for $x=100\%$ then $\epsilon=2.2\%$ also the incorporation of Manganese Mn causes a tensile strain. The figure 3 shows the variation of the strained structure's energy gap depending on the manganese

concentration x . The layer is subjected to a tensile strain, so the heavy holes' band is below the light holes' band and the absorption can be for only incident photon energy greater than 1.6eV. The figure 4 represents change of absorption coefficient as a function of energy incident light for different values of manganese concentration. The increase in the concentration of Mn leads a reduction absorption coefficient. For a photon energy $E_{ph}=3eV$, $x=20\%$ the absorption is $\alpha=1.7210^5cm^{-1}$ and for $x=50\%$ it is $\alpha_2=1.2710^5cm^{-1}$. We shows that the absorption decreases as $\Delta\alpha=0.4510^5cm^{-1}$. We also note that for $x=20\%$ the maximum absorption is $\alpha_{max}=1.8810^5cm^{-1}$ and for $x=50\%$, $\alpha_{max}=1.4610^5cm^{-1}$; we have then a decrease of $\Delta\alpha_{max}=0.4210^5cm^{-1}$. The figure 5 illustrates the variation of the refractive index as a function of manganese concentration. The refractive index of the material does not exceed value of $n=2.9$, so we can say that the reflectivity decreases with manganese concentration rising. The figure 6 shows current- voltage characteristic for several concentrations of Mn. The increasing of manganese concentration leads to a reduction of the short circuit. For $x=10\%$, $J_{cc}=65.41mA/cm^2$ and for $x=70\%$, $J_{cc}=49.95mA/cm^2$; we have then a decreasing of $\Delta J_{cc}=15.96mA/cm^2$. The figure 7 shows the variation of the power delivered by the cell as the function of bias voltage for different manganese percentages. We notice a decrease in power in accordance with the increase of x . For an 25% manganese increasing in structure, we find that there's a significant reduction of the maximum power $\Delta P=5.2mw/cm^2$. We see a reduction in cell efficiency by increasing the percentage of manganese in the active layer. For $x=0\%$ the efficiency is 20.25% and for $x=10\%$ it is 14.01. We need to find a compromise between the manganese concentration and strain to achieve a reliable structure.

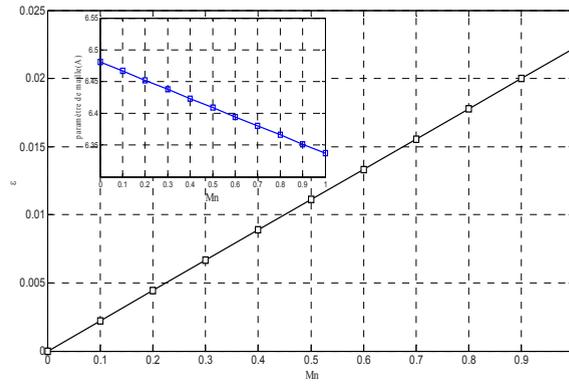


Figure 2. change mismatch versus manganese concentration in the $Cd_{1-x}Mn_xTe / CdTe$ structure.

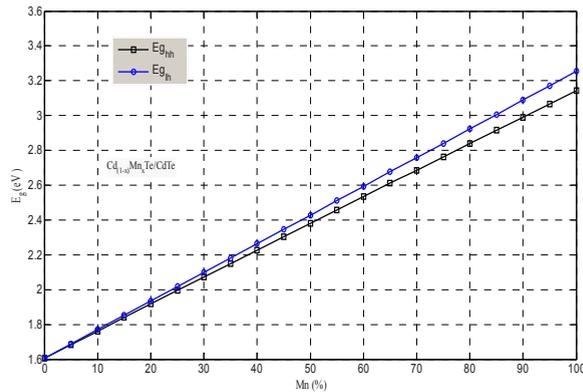


Figure 3 . band gap energy variation of the strained structure as function of manganese concentration.

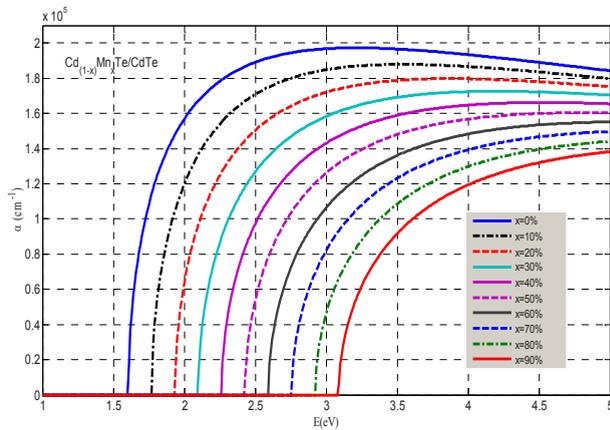


Figure 4 .variation of absorption as function of photon energy.

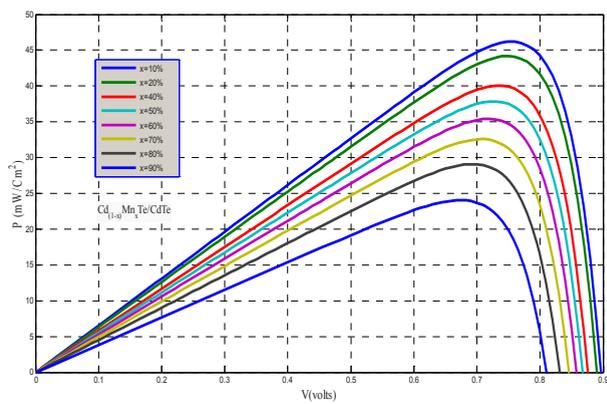


Figure 5. current-voltage characteristic of CdMnTe structure

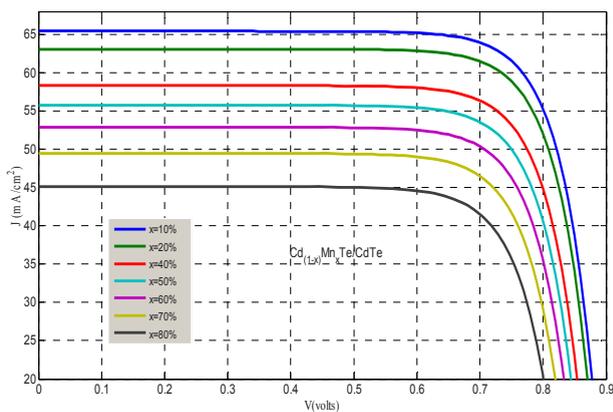


Figure 6 . power delivered by cell based on CdMnTe.

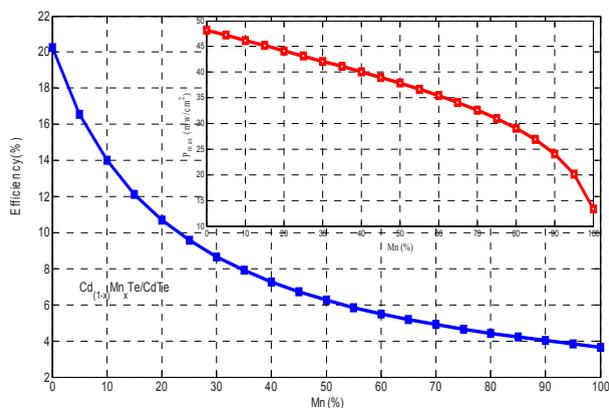


Figure 7. conversion efficiency of the cell based on CdMnTe.

5. Conclusion

This work focuses on the study and simulation of electrical characteristics of a solar cell based materials ternary $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ on a substrate CdTe ; either the effect of different physical and optical parameters of the cell has been explored. We considered the impact of manganese concentration on the physical parameters of the ternary and the strain effect between the two layers of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ and CdTe . The results show that the epitaxial alloy is under low tension strain. The increasing of manganese concentration increases the gap. For optoelectronic characteristics, the incorporation of manganese reduces the absorption coefficient. We determine the influence of Mn on the $I(V)$ characteristic and the power delivered by the cell. The obtained results allow the calculation of maximum efficiency of the cell which reaches 20 %.

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