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Modeling and simulation of the structure based on the semiconductor III-V for solar cell application

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Abstract

This work focuses on modeling and simulation of structure based semiconductors III.V for solar cell application. We first studied the influence of the concentration of indium on the various parameters of the alloy and GaInAsSb on GaAs substrate. Indeed, the increased density of indium decreases the bandgap energy of the alloy, which is very interesting to absorb maximum solar spectrum. We can obtain this structure by gap energy less than 1 eV. The study includes graphs showing the variations of the different factors affecting the conversion efficiency as a function of indium concentration and the thickness of the semiconductor layer. The most appropriate structure for this work is GaInAsSb because it has improved performance.

Keywords: strain quantum wells - GaInAsSb /GaAs ; semiconductor III-V ; solar cells

1. Introduction

The consequences of the use of fossil fuels require finding alternative sources of supply. Among the choices that meet the cost, durability and environmentally friendly, renewable energy appear to be a good compromise. They are inexhaustible energy provided by the sun, wind, falling water, the heat of the earth ... etc. Their exploitation does not generate polluting emissions. Among these energies of the future, solar photovoltaic that can convert sunlight directly into electricity occupies an important place in research, and is growing increasingly important since 1990. This research is focused on two main axis, which may seem opposite (increase cell efficiency, and reducing the cost of production) [1]. This development is mainly through the control of materials used in the design of components. Most of these materials are obtained by standard alloy on substrates. They could in principle cover a wide range of compositions and therefore application. This study is oriented towards the study and simulation of structures based on GaInAsSb / GaAs, for photovoltaic and improving the efficiency of this structure. The development of systems of photovoltaic conversion in the last thirty years has led to significant improvements in terms of cost and performance. To date the best photovoltaic conversion efficiencies are obtained with solar concentration systems using multi cell junctions based semiconductors III-V materials. The world record in this area is currently owned by the Spire with a yield of 42.3% measured on a multi-junction type GaInP / GaAs / InGaAs bifacial and a concentration factor of solar radiation 406 cell. Previously in 2009, the company Spectrolab (USA) had a return of 41.6% with cells GaInP/GaInAs/Ge [3].

2. Theory

Compounds containing bore, aluminum or nitrogen fall into this category, they generally have little interest in fast electronics, which requires semiconductors with high carrier mobility or for optoelectronics or a direct band gap structure is necessary for the optical transitions are effective. At the other end, the heavy elements such as bismuth or thallium-based compounds give Gallium (GaAs, GaSb) or indium (InP, InAs, InSb) whose properties are very interesting. Table (1) summarizes some parameters for different materials of the III-V [4].

Semicon ductor III-V	E_g (eV)	m^*/m_0	μ (cm^2/VS)	a (Å)
GaP	2,26	0,82	110 5	5,4512
GaAs	1,42	0,067	8500	5,6533
InP	1,35	0,077	4600	5,8686
GaSb	0.812	0.046	-	6.096
InAs	0,36	0,023	33000	6,0584
InSb	0.235	0.016	-	6.479

Table 1. Parameters of the main binary compounds.

The lattice constant is estimated from Vegard's law [5], i.e for a quaternary alloy type $A_xB_{(1-x)}C_yD_{(1-y)}$ is expressed by:

$$a(x,y) = x.(1-y)a_{AD} + (1-x).y.a_{BC} + x.y.a_{AC} + (1-x).(1-y)a_{BD} \quad (1)$$

$a_{AC}a_{AD}$, a_{BC} and a_{BD} are the lattice constants of the binary compounds constituting the alloy.

Epitaxy of two semiconductors of the same crystalline structure but of different lattice parameter initially, causes strain (Figure. 1). The material constituting the layer of greater thickness imposes its lattice parameter adjacent to each other of the contact interface, so for sufficiently thin layers, the lattice parameter of epitaxy material and elastically deforms according to the parameter of the layer epitaxy is smaller or larger than that of the substrate, the deformation or elongation is "relaxation layers" or narrowing "compression layer". For a description of the effect of strain on the band structure model and Van De Walle and Krijin formalism are used [6].

In the absence of stress, the bands of heavy holes and light holes are degenerated and isotropic in the center of the Brillouin zone, and the strip-splitting spin holes is located at an energy Δ_0 below these two bands. The center of gravity of the valence band average energy $E_{v,moy}$ is therefore $\frac{\Delta_0}{3}$ below the top of the valence band at k = 0.

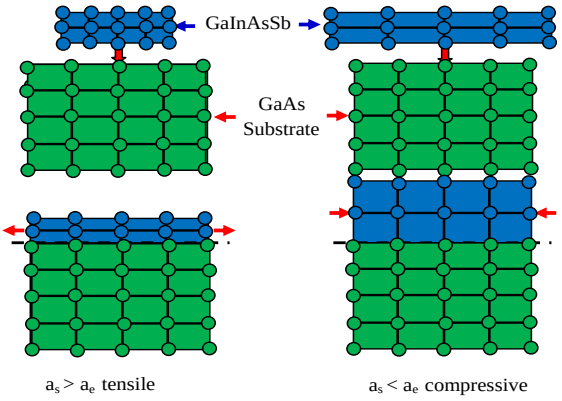

Figure 1. Two types of deformation, (a) layer in compression $a_s<a_e$ (b) layer relaxation $a_s>a_e$.

The effect of strain on the valence and conduction band can be decomposed into two parts:

- The hydrostatic stress, due to deformation along the axis of growth, causes a shift of the center of gravity of the valence band and the center of gravity of the conduction band.
- The Shear stress, which lifts the degeneracy of the energy states of the heavy hole and light hole in k = 0.

For an epitaxial layer subjected to a bi-axial compressive strain, the hydrostatic component increases the gap between the valence band and the conduction band, and the shear stress makes the valence bands strongly anisotropic .the band highest energy becomes heavy according to $k_\perp$ and light according $k_\parallel$(hh band). The lower energy band it becomes slightly according $k_\perp$ and heavy according $k_\parallel$ (lh band).
Energy shifts of the centers of gravity of the valence band and the conduction band in K = 0 induced by the hydrostatic stress, vary proportionally with stress [6]. Expression of the gap energy with duress band is given by:

$$E_g^{cont} = E_c - E_v = E_g(x,y) + \Delta E_c^{hyd} - \Delta E_{v,moy}^{hyd} - max\left(\Delta E_{hh}^{cisa}, \Delta E_{lh}^{cisa}\right) \quad (2)$$

$\Delta E_{v,moy}^{hyd}$, $\Delta E_{v,moy}^{hyd}$, ΔE_{hh}^{cisa} and$\Delta E_{lh}^{cisa}$are the offset of the conduction bands of strain and valence heavy holes and light holes, respectively.

In case the strained layer is a solid solution of quaternary form $A_x B_{x-1}C_yD_{1-y}$, these parameters can be determined by linear interpolation, except for E_g energies are determined qui $\Delta_0/3$ by the following expression:

$$Eg(x,y) = (1-x).y.E_{BC} + (1-x)(1-y).E_{Bd} + x.y.E_{AC} + x(1-y)E_{AD} - x(1-x).y.C_{ABC} - x.y(1-y).C_{ACD} - (1-x).y(1-y).C_{BDC} - (1-x).x \quad (3)$$

During the passage of light in the active layer of the photovoltaic cell, a photon can be absorbed by this layer to produce an electron-hole pair called exciton [7]. The absorption coefficient α for photon energy greater than the energy E of the gap is given by the following relationship:

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

With α_0 is constant.

3. Results and discussion

Figure 2 shows the variation of the lattice mismatch as a function of the indium (In) and antimony (Sb) concentration of the structure $Ga_{(1-x)}In_{(x)}As_{(1-y)}Sb_{(y)}$/GaAs. Note that the indium and antimony concentrations cross deformation of the structure but the influence of the indium concentration is more important than the effect of the antimony concentration. Figure.3 shows the effect of the antimony concentration in the valence band. The incorporation of Sb on GaInAs structure gives a breakdown in valence band into two bands E_{lh}^{+}, $E_{lh}^{-}$and E_{lh}^{+}, E_{lh}- heavy and light holes, respectively. This phenomenon affects the bandgap energy. Figure. 4 shows the evolution of the gap energy of heavy holes and light holes depends on the In and Sb concentration of band. It is found that the indiumand antimony concentration significantly reduces the energy bandgap E_{glh} and E_{glh}. If a couple is taken (In = 14%, Sb = 10%) the gap E_{glh} = 1 eV for the pair (In = 34%, Sb = 10%) the gap is 0.79eV E_{glh} was a decrease ΔEg = 0.21eV. Figure.5 shows the variation of the absorption of the structure according to the coefficient of In and Sb concentrations. Note that the absorption coefficient increases with increasing of both of In and Sb concentrations. So indium and antimony cross absorption GaInAsSb/GaAs structure.

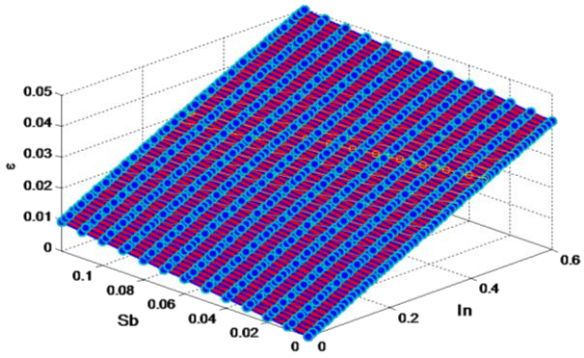

Figure 2. Variation of deformation as a function of the indium and antimony concentrations.

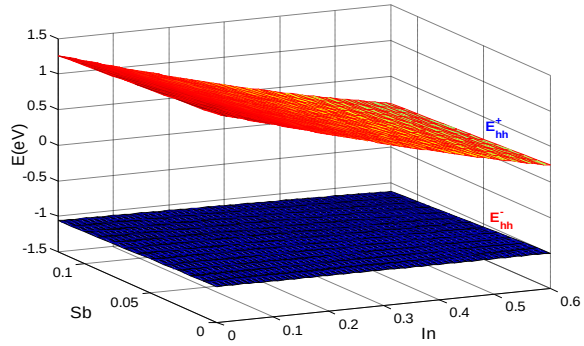

Figure 3. Variation of the energy of the valence band of heavy holes in function of the In and Sb concentrations.

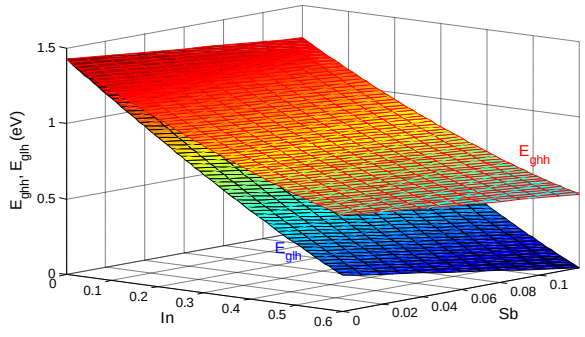

Figure 4. Variation of the gap as a function of the indium and antimony concentrations.

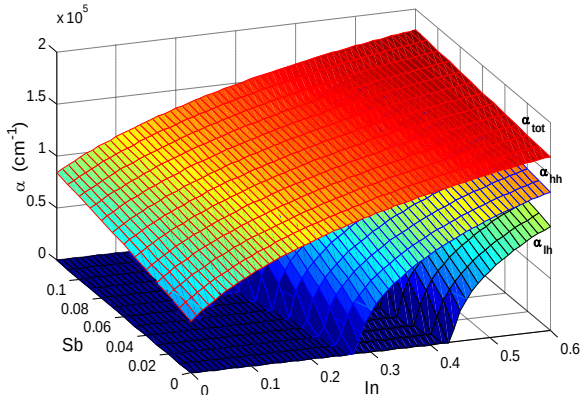

Figure 5. Variation of absorption of the different transitions elections heavy holes and light holes in total based on In and Sb concentrations.

4. Conclusion

In this work we modeled and simulated the structure based on GaInAsSb on GaAs substrate. We took into account the effect of In and Sb concentrations on the strain the energy in the valence subband, the bandgap energy and the absorption coefficient. In and Sb concentrations decreased significantly the bandgap energy is giving us a very significant increase in the absorption coefficient of the structure GaInAsSb/ GaAs. This study allows us to enhance the efficiency of light conversion .We can use this new material as one of the layers of a multi-junction solar cell.

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