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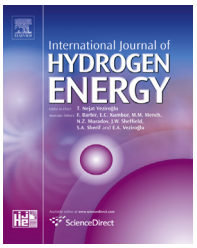

Modeling and simulation of $Al_xGa_yIn_{1-x-y}As/InP$ quaternary structure for photovoltaic

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ABSTRACT

In this work, we have studied solar cells based on AlGaInAs/InP quaternary structure to describe the behavior of electronics components. To this end, we have developed a simulation program to study the gallium Ga and aluminum Al concentrations effect on respectively the lattice mismatch, the band gap energy, the absorption and the power delivered by the solar cell. This study allows us to compare between simulation and experimental results, once the cell parameters are optimized by a judicious choice of concentrations. This work allows us either to use nanotechnologies for solar cells.

Introduction

The ecological problems induced by the use of fossil fuels that are moreover finite resources, require finding alternative energy sources. Among the choices that satisfy the cost, durability and are eco-friendly, renewable energies appear to be a good compromise. They are endless energies provided by the sun, wind, falling water etc… Their usages do not generate pollution. Among these energies of the future, solar photovoltaic energy that allows the direct sunlight conversion into electricity; occupies an important place in research and it's growing increasingly since 1990. Thus, for example, photocatalysis realized by novels semi conductor compounds for splitting water into hydrogen under visible light irradiation is an attractive method to obtain renewable hydrogen source [1,2]. The use of solar energy to generate hydrogen is expected to over 50% by using electrochemical cells and concentrated photovoltaic cells (CPV) [3]. Also the converting solar irradiation into electricity by solar cells to produce DC power can be combined with electrochemical process to produce hydrogen used for generating electrical energy [4]. This research is dividing into two main axes, which may seem opposites (increasing cell efficiency and decreasing production cost) [5,6]. This development requires a perfect mastery of the materials used in the components design. Most of these materials are obtained by alloy on standard substrates and they could cover a wide range of compositions [7–10].

Theory

Strain effect on the band gap

When the lattice parameters are slightly different, the material constituting the larger thickness layer impose its lattice to other, at least in the interface vicinity .This results to the existence, in the thin material, of a bi-axial strain in the layers plane. Fig. 1 illustrates this strain effect for two crystals. To

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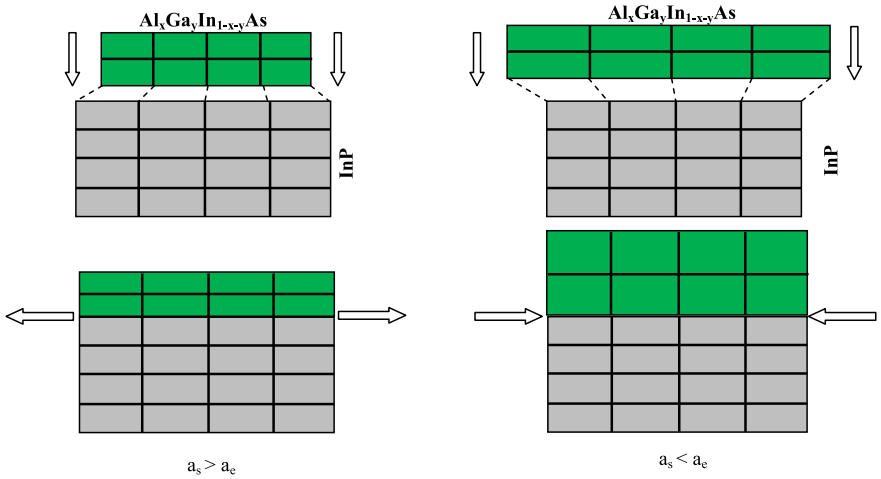

Fig. 1 – (a, b): illustration of the two types of strain: a) tensile strain b) compressive strain.

describe strain effect on the band structure we used the Van De Walle model and the Krijn formalism [11]. Both parallel and perpendicular strain tensor components can be defined as follows:

$$\varepsilon_{//} = \frac{a_{//} - a}{a} \quad (1)$$

$$\varepsilon_{\perp} = \frac{a_{\perp} - a}{a} \quad (2)$$

For a fully strained structure:

$$a_{//} = a_{sub} \quad (3)$$

$$\varepsilon_{\perp} = -2 \times \frac{C_{12}}{C_{11}} \times \varepsilon_{//} \quad (4)$$

Fig. 2 illustrates the bi-axial strain effect on the band structure of the epitaxial layer. This figure shows the band structure of a direct gap semiconductor for the three possible cases, unstrained, compressive strained and finally tensile strained. In the absence of strain, the heavy holes and light holes bands are degenerated and isotropic in the Brillouin zone center, and the spin–orbit splitting is located at energy Δ_0 below these two bands. The valence band gravity center with average energy $E_{v,moy}$ is consequently localized at $\Delta_0/3$ below the top of valence band in $k = 0$ (Fig. 2a).

$$E_{V,moy} = \frac{E_{HH} + E_{LH} + \Delta_0}{3} \quad (5)$$

where E_{HH} is the heavy holes band energy, E_{LH} the light holes band energy and Δ_0 the spin–orbit splitting band.

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

- The hydrostatic component related to the deformation along the growth axis causes a gravity center shift of both valence band and conduction band.
- The shear strain lifts the degeneracy of heavy holes and light holes energy states in $k = 0$ (typically to a Δ_{hh-lh} value of about 60–80 meV for a mismatch of 1%).

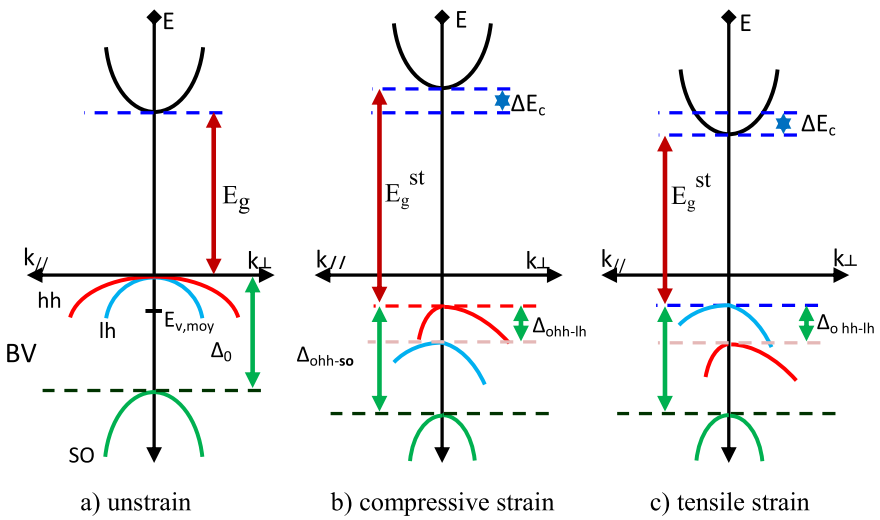

Fig. 2 – Band structure of a direct gap semiconductor.

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