The First National Conference on Renewable Energies and Advanced Electrical Engineering (NC REAEE'25)

May 06-07th, 2025

University of M'Sila

Faculty of Technology

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Authors: ***Mezrag Fadila, Bouarissa Nadir***

at the First National Conference on Renewable Energies and Advanced Electrical Engineering (NC-REAEE'25), held at M'Sila University- Algeria, on May 6–7th 2025.

Conference Chair

Dr. Abderrahim ZEMMIT

Paper ID: **219**

LGE
Laboratoire de génie électrique

University Mohamed Boudiaf - M'Sila
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Band Gap Energies of lattice matched $Ga_xIn_{1-x}As_yP_{1-y}$ quaternary alloys to InP and GaAs substrates

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Abstract

This study examines the band gap energies of zinc-blende $Ga_xIn_{1-x}As_yP_{1-y}$ quaternary alloys that are lattice-matched to InP and GaAs substrates. Utilizing theoretical modeling based on the pseudopotential approach under the virtual crystal approximation, this research explores the compositional dependence of the band gap across the full range of x and y values that maintain lattice matching. Our findings indicate that by varying the Gallium concentration, $Ga_xIn_{1-x}As_yP_{1-y}$ exhibits a direct band-gap semiconductor for all possible values of x and y ($0 \leq x \leq 0.47$, $0 \leq y \leq$ and ($0.52 \leq x \leq 1$, $0 \leq y \leq 1$) lattice-matched to InP and GaAs, respectively. This work provides valuable data for optimizing GaInAsP-based heterostructures for applications in lasers, photodetectors, and multijunction solar cells.

Keywords: Band gap energies ; Pseudopotential ; Quaternaries; GaInAsP

1. Introduction

The III–V semiconductors, are key materials for many applications, such as high-speed electronic and long-wavelength photonic devices [1–5]. The band-gap energy is known to be one of the most useful device parameters since it is strongly connected with the operating wavelength of the optoelectronic devices. Thus, the ability to calculate the band structure of alloy semiconductors is an important prerequisite for any analysis of the phenomena occurring.

In recent years, ternary and quaternary semiconductor alloys have been of great interest for the design and fabrication of the devices. By using ternary or quaternary semiconducting alloys, the band gaps and lattice constants can be continuously varied over a wide range [6–10] as a function of the alloy compositions. In the present contribution, the optical properties of $Ga_xIn_{1-x}As_yP_{1-y}$/InP have been studied using essentially the empirical pseudopotential method (EPM) within the virtual crystal approximation (VCA). The aim of the present paper is to provide a wide range of various refractive indices and high-frequency dielectric constants by simply changing the composition parameters x and y.

2. Computational method

The calculation of the electronic band structure is mainly based on the EPM within the VCA [11]. The atomic form factors have been deduced empirically by fitting the band structure to experimental data available from the literature. The empirical pseudopotential parameters are optimized using the non-linear least-squares method [12,13]. The final local adjusted symmetric V_S and antisymmetric V_A pseudopotential form factors and the used lattice constants at room temperature for GaAs, InAs GaP and InP compounds are listed in Table1.

3. Results and discussion

The formalism can be easily generalized to the case of an alloy using the VCA. In practice, V_S and V_A of an alloy can be expressed in terms of those of the binary compounds involved. Hence, for the quaternary system $Ga_xIn_{1-x}As_yP_{1-y}$ being studied here, V_S and V_A are expressed as,

$$V_S^{alliage} = xyV_S^{GaAs} + (1-x)yV_S^{InAs} + x(1-y)V_S^{GaP} + (1-x)(1-y)V_S^{InP} \quad (1)$$

$$V_A^{alliage} = xyV_A^{GaAs} + (1-x)yV_A^{InAs} + x(1-y)V_A^{GaP} + (1-x)(1-y)V_A^{InP} \quad (2)$$

The variation of the lattice constant of the quaternary alloy of interest as a function of compositions x and y is determined as,

$$a_{alliage} = xya_{GaAs} + y(1-x)a_{InAs} + x(1-y)a_{Gap} + (1-x)(1-y)a_{InP} \quad (3)$$

where $a_{GaAs}, a_{InAs}, a_{GaP}$ and a_{InP} are the lattice constants of GaAs, InAs , GaP and InP, respectively.

The lattice matching condition for $Ga_xIn_{1-x}As_yP_{1-y}$ on InP substrate is as follows

$$y = \frac{0.5431x}{0.1893 + 0.0132x} \qquad (0 \le x \le 0.7 \quad \text{and} \quad 0 \le y \le 1) \qquad (4)$$

Figure 1 displays the direct (Γ-Γ) and indirect (Γ-X) and (Γ-L) energy band-gaps of $Ga_xIn_{1-x}As_yP_{1-y}$ lattice matched to InP versus the composition x. Note that all the band gaps decrease monotonically with increasing Ga content on going from x=0 to 0.47 without showing any transition between the direct and indirect structures. One may expect thus that $Ga_xIn_{1-x}As_yP_{1-y}$ is a direct (Γ-Γ) band-gap semiconductor within the x composition range $0 \le x \le 0.47$.

The refractive index (n) of a material is the most important property of any optical system that uses refraction. It describes optical characteristics of a medium. The n of $Ga_xIn_{1-x}As_yP_{1-y}$ lattice matched to InP versus the alloy composition x has been calculated using different models, namely the Moss model [14], the Ravindra model [15], the Gupta and Ravindra model [16], the Hervé and Vandamme model [17], the Reddy and Anjaneyulu model [18], and the Reddy and Ahmmed model [19]. The obtained results showed that the best agreement with experiment (n=3.1[20]) is obtained when the model of Hervé and Vandamme (n=3.04) is used. Our data are plotted in Fig.2. Note that as the composition parameter x increases on proceeding from 0 to 0.47, n increases as well for all models used exhibiting a monotonic and non-linear behavior.

The high-frequency dielectric constant ε_∞ has also been calculated using the same relation as that used in Ref. [21],

$$\varepsilon_\infty = n^2 \qquad (5)$$

The agreement between the ε_∞ value of 9.23 obtained in this work and the experimental one of 9.61 reported in Ref. [20] is within 4%. The variation of ε_∞ for zinc-blende $Ga_xIn_{1-x}As_yP_{1-y}$ lattice matched to InP as a function of the composition x in the range 0-0.47 is shown in Fig.3. We observe that by increasing the Ga concentration, the high-frequency dielectric constant increases as well. The behavior is monotonic and nonlinear. The trend of ε_∞ suggests that for a proper choice of x, the alloy system of interest can provide more opportunities for the storage and dissipation of electric and magnetic energy in the material under study.

4. Summary

The optical properties of $Ga_xIn_{1-x}As_yP_{1-y}$ quaternary alloys lattice matched to InP have been investigated using the EPM under the VCA. A summary of the key findings follows:

(i). The direct (Γ-Γ) band-gap energy of $Ga_xIn_{1-x}As_yP_{1-y}$ quaternaries lattice matched to InP exhibits a monotonic and non-linear behavior with the composition parameter x.

(ii). Lattice matched to InP substrate $Ga_xIn_{1-x}As_yP_{1-y}$ is found to be a direct band-gap semiconductor for all possible values of x and y ($0 \leq x \leq 0.47$, $0 \leq y \leq 1$).

(iii). More opportunities for the storage and dissipation of electric and magnetic energy were found when varying the composition x $Ga_xIn_{1-x}As_yP_{1-y}$/InP.

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Figure captions

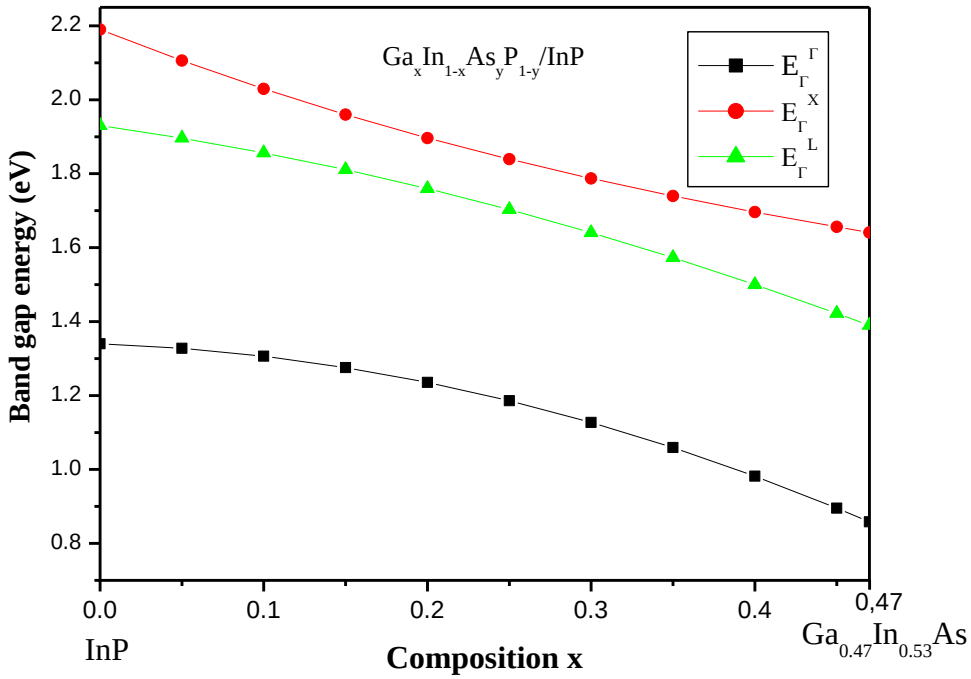
Fig.1. Direct (Γ-Γ) and indirect (Γ-X) and (Γ-L) energy band-gaps in $Ga_xIn_{1-x}As_yP_{1-y}$ lattice matched to InP versus composition parameter x.

Fig.2. Refractive index in $Ga_xIn_{1-x}As_yP_{1-y}$ lattice matched to InP versus composition parameter x.

Fig 3. High-frequency dielectric constant in $Ga_xIn_{1-x}As_yP_{1-y}$ lattice matched to InP versus composition parameter x.

Table 1. Pseudopotential parameters for GaAs, InAs , GaP and InP

Compound	Form factors (Ry)						Lattice constant (A^0)
	$V_S(3)$	$V_S(8)$	$V_S(11)$	$V_A(3)$	$V_A(4)$	$V_A(11)$	
GaAs	-0.200313	0.00	0.068396	0.106112	0.06	0.03	5.8687
InAs	-0.214015	0.00	0.046505	0.045385	0.045	0.01	6.0583
GaP	-0.225284	0.00	0.109755	0.084005	0.06	0.03	5.4505
InP	-0.235393	0.0126	0.057018	0.073883	0.05	0.01	5.6533


Ga$_x$In$_{1-x}$As$_y$P$_{1-y}$/InP
E_Γ^Γ
E_Γ^X
E_Γ^L
Band gap energy (eV)
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.0
0.1
0.2
0.3
0.4
0,47
InP
Composition x
$Ga_{0.47}In_{0.53}As$

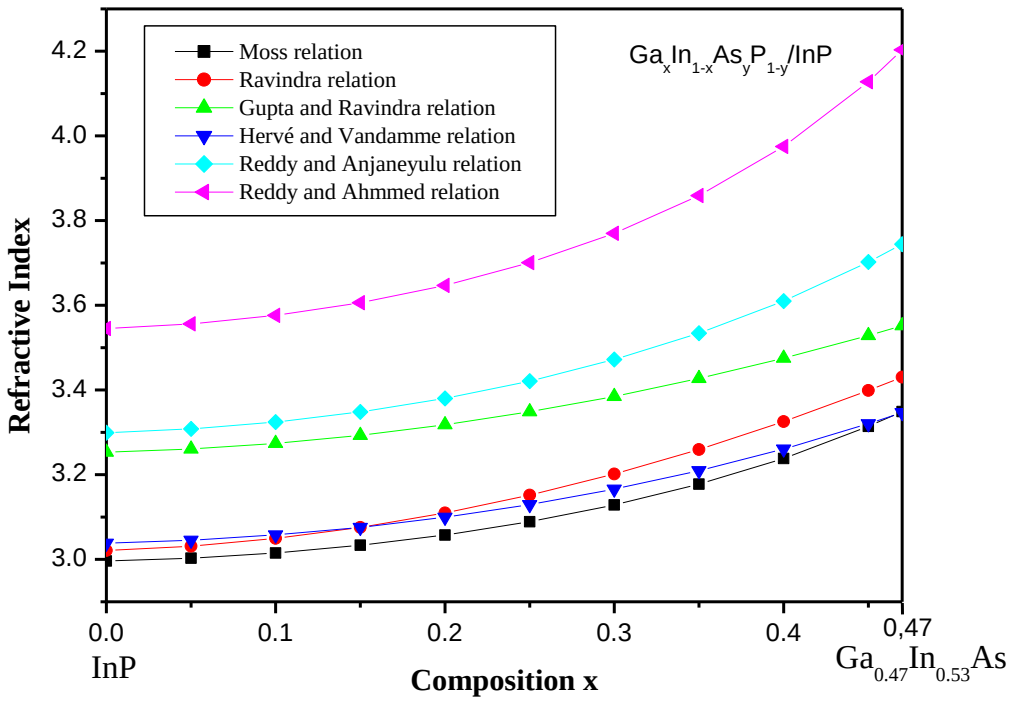

Moss relation
Ravindra relation
Gupta and Ravindra relation
Hervé and Vandamme relation
Reddy and Anjaneyulu relation
Reddy and Ahmmed relation
Ga$_x$In$_{1-x}$As$_y$P$_{1-y}$/InP
Refractive Index
4.2
4.0
3.8
3.6
3.4
3.2
3.0
0.0
0.1
0.2
0.3
0.4
0,47
InP
Composition x
$Ga_{0.47}In_{0.53}As$

Figure1.

Figure 2.

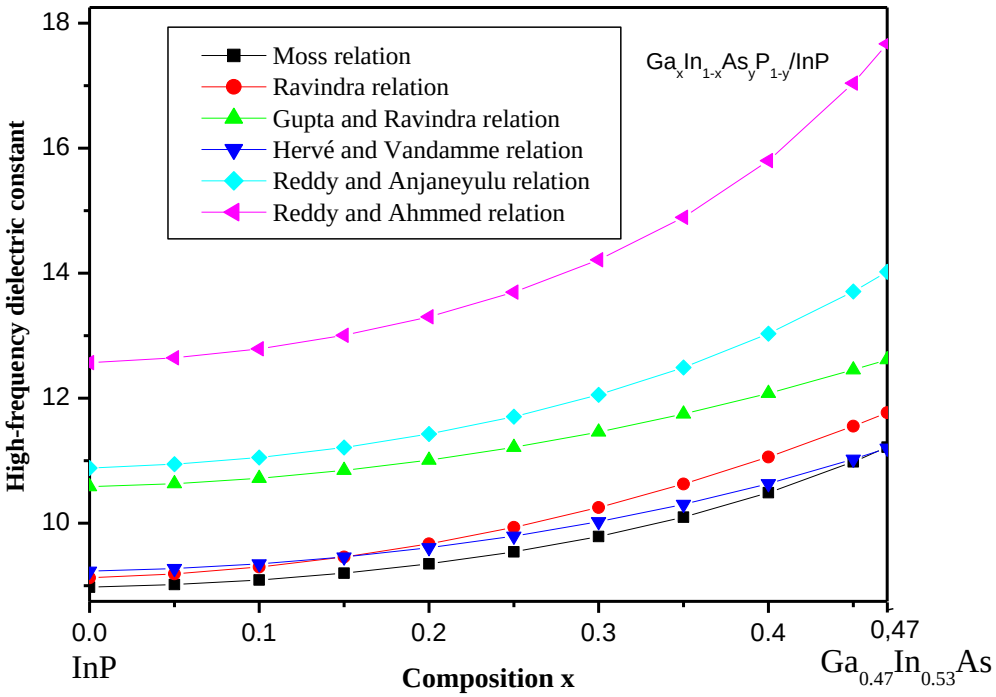


Figure 3.