Quantum Mechanical Study on Material Parameter Aspects of $Ga_xIn_{1-x}As_yP_{1-y}$ Quaternary System Grown on InP Substrate

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A formalism based on quantum mechanical concepts has been used to study the material parameter aspects of GaInAsP quaternary system grown on InP. Results pertaining to the lattice match internal strain, band-gap and refractive index are presented.

INTRODUCTION

The study on micro-optoelectronic material parameters is of much technological importance and use to the materials and device engineer in engineering the material properties. Tailoring (band-gap engineering) of these parameters are of vital for the growth and fabrication of multi-layered device structures for specific and strategic high-end applications. The feed back from these studies provides valuable insights and clues for fabricating structures with controlled properties. The factors which influences the properties of the hetero-epitaxial multi-layered structures based systems include lattice mis-match, strain, and band gap and refractive index. Moriizumi and Takahashi [1] have developed a procedure to identify the compositional conditions required for good lattice match with GaAs substrate using Pauling's tetrahedral radii in Vegard's law. Mani et al [2] have extended the procedure to other III-V binary substrates. Nahory et al [3] have reported the measurements of some material properties of $In_{1-x}Ga_xAsyP_{1-y}$ grown on InP over a compositional range for lattice matched material ($0 \leq x \leq 0.47$, $0 \leq y \leq 1$). The pioneering works [4,5] gives the well-documented review on the band gap. Refractive indices of III-V alloys have been reviewed in ref. [6].

ROLE OF LATTICE MATCH IN FORMATION OF HETRERO-JUNCTIONS

The nature of chemical bonding plays an important role in the formation of hetero-junction. In III-V compounds the bonds are covalent and hence the present study, Pauling's tetrahedral radii (THR) are used. In zinc-blende structure, each atom is surrounded tetrahedrally by four other atoms; characteristic radii can be assigned to each atom, such that the separation between the nuclei of the neighboring atoms (interatomic distance) is the sum of the two atomic radii. The inter-atomic distance (ID) of the III-V compounds is equal to the lattice constant times $\sqrt{3}/4$ A). If the substrate crystal is given, the alloy to be grown must be selected so as to obtain a good lattice match, because good lattice match correspondence to good ID matches. For that, the following condition must be fulfilled.

$$\sum_{m=1}^{3} a_m x_m + \sum_{n=1}^{3} b_n y_n = ID_{substrate} \qquad (1)$$

THE GaInAsP-InP LATTICE-MATCHED STRUCTURE

The GaInAsP quaternary system is bounded by the InAsP, GaInAs and GaAsP ternaries. The key advantage of this system is that, two commercially available substrates GaAs and InP can be employed for the epitaxial growth of lattice-matched quaternary layers. When InP is used as a substrate, lattice matched GaInAsP alloys can be prepared whose band gaps span the energy between 0.75 and 1.35 eV.

GaInAsP ALLOY LATTICE MATCHED TO InP SUBSTRATE

Olsen et al [7] have grown $In_{1-x}Ga_xAs_yP_{1-y}$ alloy (Vapor Phase Epitaxy) on to InP substrate and measured the chemical compositions using electron microprobe analysis. For our numerical analysis, we have considered the same system. For this alloy system $x_1 = y_3 = 0$ (i.e., the alloy contains neither Al nor Sb)

$$(b_2-b_1)y_2=(a_3-a_2)x_2. \quad (2)$$

Using the values of a_2, a_3, b_1 and b_2 in eqn.[2], the composition of the alloy lattice matched to InP substrate, is found to be [8]

$$Ga_xIn_{1-x}As_{2.25x}P_{1-2.25x} \quad (3)$$

Antypas et al [9] developed a model for good lattice match of quaternary InGaAsP layers to InP substrate and found optimum composition as

$$Ga_xIn_{1-x}As_{2.18x}P_{1-2.18x} \quad (4)$$

Nahory et al [3] have shown the conditions for good lattice match between the alloy and InP substrate on the basis of constituent binary data. Lattice parameters of the quaternary alloy have been deduced from the binary data and compared with the measured values. The experimentally reported composition for good lattice match is

$$Ga_xIn_{1-x}As_{2.15x}P_{1-2.15x} \quad (5)$$

The compositions of the alloys grown on InP substrate cab be calculated using equations [3,4,5]. The inter-atomic distance of $Ga_xIn_{1-x}As_yP_{1-y}$ quaternary alloy grown is

$$ID = 1.26x_2 + 1.44\,(1-x_2) + 1.10\,(1-y_2) + 1.18y_2 \quad (6)$$

The lattice constant of the grown alloy is calculated for different experimentally measured compositions and compared with result [2].

STRAIN IN THE QUARTERNARY COMPOUNDS

Preparation of ternary and quaternary materials from respective III-V binaries leads to an internal strain in the ternary or quaternary material due to the differences of lattice constant of the binary compounds resulting in the crystal lattice deformation. Sonomura et al [4] have estimated the internal strain in the $Ga_xIn_{1-x}As_yP_{1-y}$ quaternary compound lattice matched to GaAs and InP substrates based on the Vegard's law. Following the equation proposed by Sonamura, the strain in the $Ga_xIn_{1-x}As_yP_{1-y}$ quaternary compound, lattice matched to InP can be written as

$$\sigma_s(x, y) = 4/\sqrt{3}\,[\{f_1\,[a_2 + b_2 - ID_{alloy}(x, y)^2 + \{f_3\,[a_2 + b_3 - ID_{alloy}(x, y)^2 + \{f_4[a_3 + b_3 - ID_{alloy}(x, y)^2]^{1/2} \quad (7)$$

Where $\sigma_s(x, y)$ is the magnitude of the strain in the quaternary having composition of x and y and a_2, a_3, b_3 are the tetrahedral radii of Ga, In, As and P respectively. The co-efficient f_1, f_2, f_3 and f_4 are the fractions of the constituent compounds GaAs, GaP, InAs and InP in the compound.

The inter-atomic distance of the $Ga_xIn_{1-x}As_yP_{1-y}$ quaternary system can be written from THR data.

$$ID_{alloy}=2.54 - 0.18x - 0.08y \quad (8)$$

and using the binary data, the ID (alloy) can also be written as

$$ID_{alloy}=1.26x_2+1.44(1-x_2)+1.10(1-y_2)+1.18y_2 \quad (9)$$

The fraction f_1, $f2$, $f3$ and f_4 are related to the composition factors x and y as follows:

$$f_1 + f_2 = x,\ f_1 + f_3 = y,\ f_1 + f_4 = 1\text{-}x \text{ and } f_2 + f_4 = 1\text{-}y \quad (10)$$

The value of x, y, f_1, f_2, f_3 and f_4 must lie between 0 and 1, as also the following relations should be satisfied.

$$\max(0, -1 + x + y) \le f_1 \le \min(x, y),$$
$$\max(0, x-y) \le f_2 \le \min(x, 1-y)$$
$$\max(0, -x + y) \le f_3 \le \min(1-x, y) \text{ and}$$
$$\max(0, 1-x-y) \le f_4 \le \min(1-x, 1-y) \quad (11)$$

The maximum value f1 is denoted by f_1 (max) as

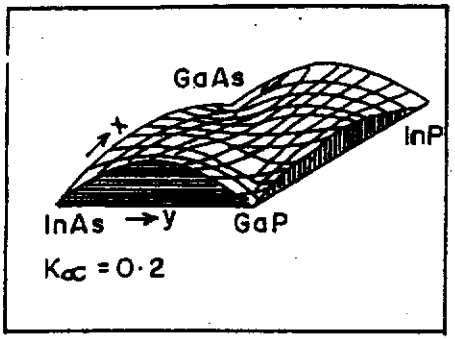

Fig.1. Strain surface of $Ga_{1-X}In_XAs_YP_{1-Y}$ for $K_{\alpha c}$ = 0·2.

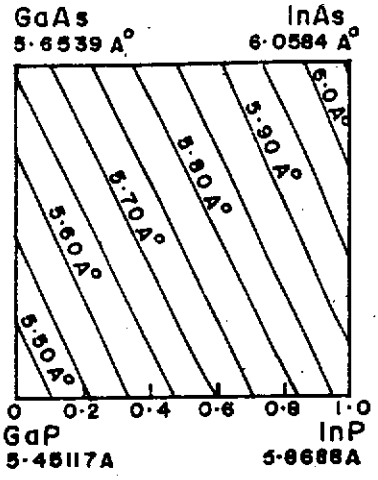

Fig.2. Isolattice constant diagram of $Ga_{1-X}In_XP_{1-Y}As_Y$ system

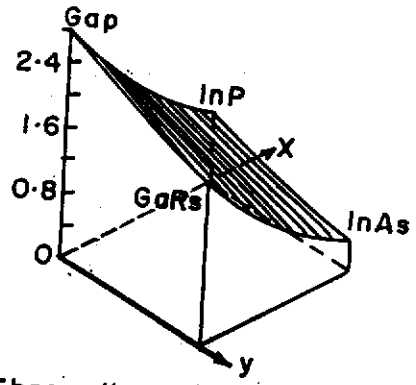

Fig.3. Three dimensional representation of the $Ga_{1-X}In_XP_{1-Y}As_Y$ direct bandgap surface.

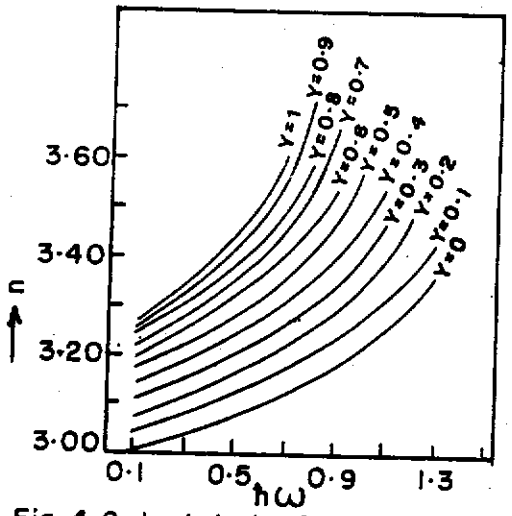

Fig.4. Calculated refractive indices of $In_{1-X}Ga_XAs_YP_{1-Y}$ as a function of the photon energy.

f_i (max) = min (x, y) (12)

The minimum value fl, f_l (min) i.e.,

f_l (min) = max (0, -1 + x + y) (13)

The value f_l can be written as

$f_l = k_\alpha (f_l \max - f_l \min) f_l \min$ (14)

The parameter f_2, f_3 and f_4 are given by

$f_2 = x - f_l$, $f_3 = y - f_l$, $f_4 = 1-x-y+f_l$ (15)

Computer simulation studies have been made and the internal strain has been visualized. Fig.1 show the three dimensional representation of the strain in the $Ga_xIn_{1-x}As_yP_{1-y}$ system. The k_α is the ratio of actual InP bonds with the maximum number of that possible in the compound. Shape of the strain surface is seen to depend strongly on the parameter k_α, when k_α is small the shape is convex, while it changes to concave as k_α becomes close to unity.

BAND ENERGY CONTOUIRS OF III-V QUATERNARY ALLOYS

The physical properties contained in the electronic structure of the III-V ternary, quaternary alloys lattice matched to III-V binary substrates are of additional importance because, these material systems provide a unique testing ground for the theoretical understanding of how these fundamental electronic properties vary with the chemical composition of a semiconductor alloy. For the direct band-gap, for ternary system,

$T_{ij}(x) = xB_j + (1-x)B_i - C_{ij}x(1-x)$, (16)

Where C_{ij} is the bowing parameter for the ternary alloy and T_{ij}, B_i and B_j are bandgap parameters. The bowing parameters of the ternary systems have been taken from the literature [10]. The iso-bandgap and direct bandgap surfaces of the GaInAsP quaternary are shown in Fig. 2 and 3.

REFRACTIVE INDEX OF GaInAsP

The lattice matching condition for the quaternary to InP substrate is

$x = 0.466\, y \quad (0 < y < 1.0)$

$m_n = xy\, m_n$ (GaAs)+ $x(1-y)\, m_n$ (GaP) + $y(1-x)\, m_n$ (InAs)+$(1-x)(1-y)\, m_n$ InP

$m_p = xy\, m_p$ (GaAs)+ $x(1-y) m_p$ (GaP) + $y(1-x)\, m_p$ (InAs)+$(1-x)(1-y)\, m_p$ InP

Where m_n is the electron effective mass, m_p is the whole effective mass and the data have been taken from [10]. Fig.4. shows the refractive index of GaInAsP as a function of photon energy and different mole fraction y.

CONCLUSION

Material parameters aspects such as lattice match, internal strain, band-gap and refractive index for typical GaInAsP quaternary system using quantum mechanical concepts have been studied and the results are presented.

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