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Optoelectronic properties of $GaAs_{1-x}P_x$ alloys under the influence of temperature and pressure

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ABSTRACT

This work is concerned with the dependence of the electronic energy band structures for $GaAs_{1-x}P_x$ alloys on temperature and pressure that is based on local empirical pseudo-potential method. The band structures of $GaAs_{1-x}P_x$ alloys were calculated in the virtual crystal approximation using the EPM which incorporates compositional disorder as an effective potential.

It was found that temperature and pressure dramatically change the crossover energies, refractive index and dielectric constant of the alloys.

The calculated energy band gaps, bowing parameters, refractive indices, and dielectric constants of $GaAs_{1-x}P_x$ alloys with different phosphide concentrations are found in close agreement with the published data.

Therefore it can be stated that the temperature and pressure are highly significant when studying and operating devices based on $GaAs_{1-x}P_x$ alloys.

1. Introduction

Semiconductor alloys play an important role in the nanotechnology science and incorporate in the fabrication of many electronic and optoelectronic devices. The recent development and advances in the epitaxial growth techniques such as molecular beam epitaxy (MBE), metal organic chemical vapor deposition (MOCVD), and other modern growth techniques [1–5], made it possible to invent new materials based on atomic and nanometer scales. These new man made materials can be prepared to achieve specific purposes for their potential applications in the industrial electronic devices.

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Gallium arsenide phosphide $GaAs_{1-x}P_x$ alloys have attracted great attention experimentally [6–9] and theoretically [10,11] for their applications in optoelectronic devices such as light emitting diodes (LED's), photo detectors, data storage, and multi-junction solar cells [12].

The band parameters, optoelectronic properties, temperature, and pressure dependence of the energy gaps in semiconductors have been the subject of many studies [13–30].

For these reasons we are interested in studying the effects of temperature and pressure on the electronic band structure and some optoelectronic properties, specifically, the energy band gaps, refractive index, and dielectric constant at the high symmetry points for $GaAs_{1-x}P_x$ alloys. Our calculations are based on the local empirical pseudopotential method (EPM) that considers the virtual crystal approximation in which the effect of compositional disorder is involved. The present calculations are performed by a routine based on the MATLAB language [31].

2. Theory and calculations

The alloy potential, $V(r)$ for $GaAs_{1-x}P_x$ alloy is calculated within the virtual crystal approximation, $V_1(r)$ which is a periodic potential and a non-periodic potential, $V_2(r)$ due to the compositional disorder [21,32,33] as

$$V(r) = V_1(r) + V_2(r) \tag{1}$$

where

$$V_1(r) = xV_{GaP}(r) + (1-x)V_{GaAs}(r) \tag{2}$$

and

$$V_2(r) = -\delta\sqrt{x(1-x)}[V_{GaAs}(r) - V_{GaP}(r)] \tag{3}$$

where δ is treated as an adjustable parameter which equals to zero when the disorder effect is neglected, and x is the phosphide, P concentration.

The potential $V(r)$ can be expanded in terms of the reciprocal lattice vectors, $\vec{G}$ as [25,29]

$$V(r) = \sum_{\vec{G}\neq\vec{G}'} a_{n,\vec{k}}(\vec{G})[W^S(\Delta\vec{G})\cos(\Delta\vec{G}\cdot\vec{\tau}) + iW^A(\Delta\vec{G})\sin(\Delta\vec{G}\cdot\vec{\tau})] \tag{4}$$

where W^S and W^A are the symmetric, S, and anti-symmetric, A, form factors, respectively, $\Delta\vec{G} = \vec{G} - \vec{G}', \vec{G}$ and $\vec{G}'$ are the reciprocal lattice vectors. $\vec{\tau} = \frac{a}{8}(1,1,1)$ is the position vector of each atom in the unit cell and a is the lattice constant.

The pseudo-potential form factors for the $GaAs_{1-x}P_x$ alloys are taken as [21,32,33]

$$W^{S,A} = xW^{S,A}_{GaP} + (1-x)W^{S,A}_{GaAs} - \delta\sqrt{x(1-x)}\left[W^{S,A}_{GaAs} - W^{S,A}_{GaP}\right] \tag{5}$$

where $W^{S,A}_{GaAs}$ and $W^{S,A}_{GaP}$ are the symmetric and anti-symmetric form factors of the pure GaAs and pure GaP, respectively.

The lattice constant of the alloy is obtained according to the relation [34]

$$a_{GaAs_{1-x}P_x} = (1-x)a_{GaAs} + xa_{GaP} \tag{6}$$

where a_{GaAs} and a_{GaP} are the lattice constants of the pure GaAs and GaP semiconductors, respectively.

The electronic energy band structure for GaAs and GaP are calculated using the local EPM. The form factors are adjusted to match the corresponding experimental values for the high symmetry points in the Brillouin zone.

Once the associated semiconductor potentials are determined, the calculations are performed to solve the band structure. The eigenvalues and the eigenvectors are found by solving the following matrix equation [29]

$$\frac{\hbar^2}{2m}|\vec{k}+\vec{G}'|^2 A_{n,\vec{k}}(\vec{G}',x) + \sum_{\vec{G}\neq\vec{G}'} A_{n,\vec{k}}(\vec{G}',x)V(|\vec{G}-\vec{G}'|,x) = E_{n,\vec{k}}(x)A_{n,\vec{k}}(\vec{G}',x) \tag{7}$$