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Electronic and optical properties of $InAs_{1-x}P_x$ alloys under the effect of temperature and pressure

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ABSTRACT

The calculations are based on local empirical pseudo-potential method (EPM) coupled with the virtual crystal approximation (VCA) which incorporates compositional disorder as an effective potential. This work is concerned with the dependence of the electronic energy band structures for $InAs_{1-x}P_x$ alloys on temperature and pressure. Some physical quantities such as band gaps, bowing parameters, refractive indices, and high frequency dielectric constants of the considered alloys with different phosphide concentration were calculated and their variations with the temperature and hydrostatic were studied. There is a good agreement between our results and the available experimental data for the binary compounds which may be a support for the results of the ternary alloys.

1. Introduction

Semiconductor alloys play an important role in nanotechnology science and fabrication of many electronic and optoelectronic devices. The Groups III–V semiconductors are compounds made between elements of Group III, such as indium, and Group V atoms such as arsenic, and phosphorus. All the compounds of interest for device manufacture have the zinc-blende crystal structure, where in each Group III atom has four Group V atoms as their nearest neighbors, and vice versa [1]. The optoelectronic properties of the semiconductor alloys are essential in the design and fabrication of devices [2]. In the design and analysis of these devices, the optical electronic energy levels, the refractive indices and the optical dielectric constants of the material of interest have to be known as a function of composition and wavelength [2].

The energy band gaps and their behavior under effect of pressure and temperature would enable us to predict overall properties of the materials of interest [3]. Several methods have been developed to calculate the band structure of semiconductors such as empirical pseudo-potential method [4–6]. In the empirical pseudo-potential method, the core electrons are tightly bound to their nuclei and the valence electrons are influenced only by a weak net effective potential called pseudo-potential, i. e. the large attractive core potential energy of the ion core is canceled by the large positive kinetic energy of the electron due to its rapid oscillations [7–10]. Dependence of energy band gaps and electronic properties for semiconductors on pressure and temperature has been investigated in several studies [11–26].

In the present study, the electronic band structure and some optoelectronic properties such as energy band gaps, refractive indices, and high frequency dielectric constants were calculated for the considered alloy. The calculations were performed by using the local empirical pseudo-potential method. The alloy potential was calculated within the virtual crystal approximation including the disorder effect. The effect of composition factor (x) from (0 to 1), temperature from (0 K to 500 K) and hydrostatic pressure from (0 Pa to 12×10^9 Pa) on the electronic band structure were studied. The calculated results at some high-symmetry points [L, Γ, X] of the binary alloys were compared with the experimental data and showed good agreement. For the other ternary alloys, where comparison with literature data was not possible, our results are predictions and may serve for a reference. The present calculations were performed by a routine based on the MATLAB language (Matlab, Mathworks Inc., Natick. Massachusetts, U.S.A.) [27].

2. Theory and calculations

The electronic structure of the alloys $InAs_{1-x}P_x$ was calculated using the empirical pseudo-potential method [28,29]. The alloy potential was determined using the virtual crystal approximation $V_{VCA}(\mathbf{r})$ which is a periodic potential beside a non-periodic potential $V_{dis}(\mathbf{r})$ due to the compositional disorder [28,29].

$$V(\mathbf{r})_{alloy} = V_{VCA}(\mathbf{r}) + V_{dis}(\mathbf{r}), \qquad (1)$$

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Table 1
The adjusted symmetric and anti-symmetric form factors and lattice constants of $InAs_{1-x}P_x$ alloy at T = 0 K, and $\mathcal{P}$ = 0 Pa for different phosphide concentrations.

x Form factors (a. u.)	0 (InAs)	0.1	0.3	0.5	0.7	0.9	1 (InP)
w_3^s (T)	−0.105375	−0.106042	−0.107796	−0.109661	−0.111606	−0.113662	−0.114900
w_8^s (T)	0.0001	0.000450	0.001371	0.002350	0.003371	0.004450	0.005100
w_{11}^s (T)	0.023791	0.024113	0.024961	0.025862	0.026802	0.027796	0.028394
w_3^a (T)	0.022674	0.023544	0.025832	0.028266	0.030803	0.033485	0.035100
w_4^a (T)	0.022494	0.022676	0.023156	0.023667	0.024199	0.024761	0.025100
w_{11}^a (T)	0.004974	0.004983	0.005006	0.005031	0.005056	0.005084	0.005100
a (a.u.)	11.430863[a]	11.395207[b]	11.323894[b]	11.252582[b]	11.181269[b]	11.109956[b]	11.074300[a]

[a] Ref. [11].
[b] Ref. [30].

where, the two potentials in Eq. (1) have the forms [28,29]

$$V_{VCA}(\mathbf{r}) = xV_{InP}(\mathbf{r}) + (1-x)V_{InAs}(\mathbf{r}), \tag{2}$$

$$V_{dis}(\mathbf{r}) = -\Omega\sqrt{x(1-x)}[V_{InAs}(\mathbf{r}) - V_{InP}(\mathbf{r})], \tag{3}$$

where, x is the phosphide concentration (P), Ω is treated as an adjustable parameter which simulate the disorder effect, its value varies from one alloy to another and equals to zero when the disorder effect is neglected. The potential V(**r**) of the associated binary compounds InAs and InP could be expanded in terms of reciprocal lattice vectors **G** as [4].

$$V(\mathbf{G}) = \sum_{\mathbf{G}\neq\mathbf{G}'} a_{n\mathbf{k}}\left(\mathbf{G}'\right)\left[W^S(\Delta\mathbf{G})\cos(\Delta\mathbf{G}.\boldsymbol{\tau}) + iW^A(\Delta\mathbf{G})\sin(\Delta\mathbf{G}.\boldsymbol{\tau})\right], \tag{4}$$

where, W^S and W^A are the symmetrical and anti-symmetrical form factors, respectively, $\Delta\mathbf{G} = \left|\mathbf{G}-\mathbf{G}'\right|$, $\boldsymbol{\tau}$ = a/8(1, 1, 1) is the position vector of each atom in the unit cell and a is the lattice constant. The energy eigenvalues of the associated binary alloys InP and InAs were calculated by solving the secular determinant Eq. [4,23].

$$\left\|\frac{1}{2}\left|\mathbf{k}+\mathbf{G}'\right|^2 - E_{nk} + \sum_{\mathbf{G}\neq\mathbf{G}'} V\left(\left|\mathbf{G}-\mathbf{G}'\right|\right)\right\| = 0. \tag{5}$$

The matrix will be a 65 × 65 matrix where the first terms of Eq. (9) give the diagonal elements of the matrix and the second terms give the off-diagonal terms. These off-diagonals are simplified in that we only need to calculate the elements for which for the zinc-blende structure and for the diamond structure which satisfy the condition, as we only use the first three non-zero pseudo-potentials [4]. The higher terms are set to zero using the assumption that the pseudo-potential is smooth into the core region where the strong repulsive and attractive potentials of the true crystal potential nearly cancel. The energy gaps of the considered alloys were determined by arranging these eigenvalues and set the top of the valence band to zero energy. The calculated energy gaps were compared with the experimental data at some high symmetry points L [0.5, 0.5, 0.5], Γ [0, 0, 0] and X [0, 0, 1] in the Brillouin zone (BZ). The form factors were adjusted until the calculated energy gaps match the corresponding experimental values. Once the accurate form factors of the associated binary alloys were defined, the form factors of the ternary alloy $InAs_{1-x}P_x$ were calculated from [28,29]

$$W^{S,A}_{InAs_{1-x}P_x} = xW^{S,A}_{InP} + (1-x)W^{S,A}_{InAs} - \Omega\sqrt{x(1-x)}\left[W^{S,A}_{InAs} - W^{S,A}_{InP}\right]. \tag{6}$$

Table 2
The calculated direct and indirect energy band gaps for $InAs_{1-x}P_x$ alloys at T = 0 K, and $\mathcal{P}$ = 0 Pa.

Composition	E_g^Γ(eV)	E_g^X(eV)	E_g^Γ(eV)
x = 0 (InAs)	1.1064,1.133[a],1.45[b]	1.3101,1.433[a], 2.1[b]	0.4170,0.417[a], 0.417[c], 0.43[d], 0.5[b]
$InAs_{0.9}P_{0.1}$	1.1561	1.3600	0.4848
$InAs_{0.7}P_{0.3}$	1.3007	1.5134	0.6695
$InAs_{0.5}P_{0.5}$	1.4553	1.6789	0.8664
$InAs_{0.3}P_{0.7}$	1.6163	1.8520	1.0716
$InAs_{0.1}P_{0.9}$	1.7869	2.0364	1.2889
x = 1 (InP)	1.8938,2.014[a], 2.25[b]	2.1544,2.384[a], 2.10[b]	1.4220,1.4236[a], 1.422[c], 1.42[d], 1.45[b]

[a] Ref. [11].
[b] Ref. [5].
[c] Ref. [26].
[d] Ref. [35].

To calculate the potential of the considered ternary alloy we used the adjusted form factors of the associated binary alloys InP and InAs. The potential of the ternary alloy has a parameter Ω which adjusted to gives good fitting with the available experimental data. This parameter Ω is independent on the form factors. It is found that the parameter Ω which is independent on the form factors has a value 0.1 to achieve good agreement. The lattice constant of the considered ternary alloys was taken according to Vegard's rule [30], as

$$a_{InAs_{1-x}P_x} = (1-x)a_{InAs} + xa_{InP}. \tag{7}$$

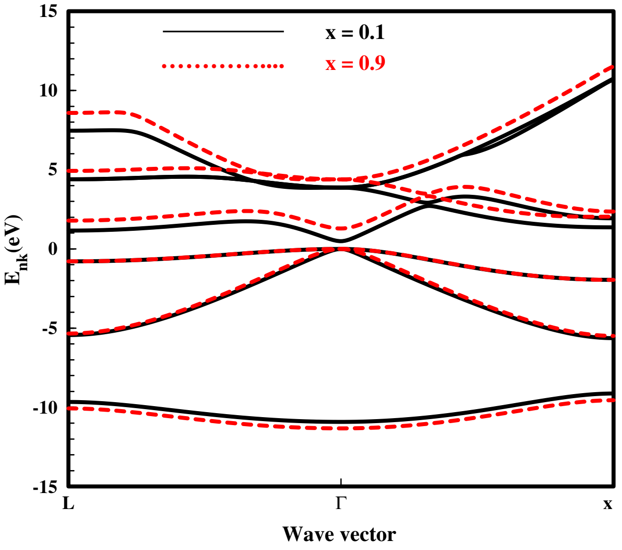

Fig. 1. The electronic structure of $InAs_{1-x}P_x$ at T = 0 K and $\mathcal{P}$ = 0 Pa for two different values of phosphide concentrations, x = 0.1 (solid line) and x = 0.9 (dashed line).