The response of temperature and hydrostatic pressure of zinc-blende $Ga_xIn_{1-x}As$ semiconducting alloys

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The electronic band structure of $Ga_xIn_{1-x}As$ alloy is calculated by using the local empirical pseudo-potential method including the effective disorder potential in the virtual crystal approximation. The compositional effect of the electronic energy band structure of this alloy is studied with composition x ranging from 0 to 1. Various physical quantities such as band gaps, bowing parameters, refractive indices, and high frequency dielectric constants of the considered alloys with different Ga concentrations are calculated. The effects of both temperature and hydrostatic pressure on the calculated quantities are studied. The obtained results are found to be in good agreement with the available experimental and published data.

Keywords: temperature, hydrostatic pressure to $Ga_xIn_{1-x}As$ alloys

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1. Introduction

The production of crystals is increased annually due to the high demand for industrial crystals based on semiconductor materials, fabricated for high technology electronic devices.[1,2] Semiconductor alloys play an important role in designing the material properties by selecting appropriate alloy constituents. Therefore, studying the band structures of semiconductor materials reveals not only the physical and electronic properties of semiconductors, but also their vital role in high speed electronic devices and nanotechnology. Many theoretical and experimental investigations into the electronic energy bands of semiconductors have been performed over the few last decades.

Ternary alloys of III–V compounds have the advantage that a considerably wide range of band gaps can be obtained by changing their alloy compositions. There is a considerable interest in the study of ternary alloy semiconductors such as $Ga_{1-x}Al_xAs$, $GaAs_{1-x}P_x$, $In_{1-x}Ga_xP$, $Ga1_{-x}In_xSb$, $Ga_{1-x}In_xAs$, etc. with the ultimate object of providing device materials with a specific band gap and band structure.[3] The ternary semiconductor alloy $Ga_xIn_{1-x}As$ with parent compounds GaAs and InAs is very attractive and plays a great role for applications in microelectronic devices.[4]

A number of studies of the structural properties of zinc-blend GaAs and InAs pure compounds have been reported,[5−12] but only a few data are available for the ternary alloy $Ga_xIn_{1-x}As$.[4]

The structural parameters of the alloy of interest are responsible for the efficiency of optical devices. Hence, an accurate knowledge of structural properties is very important.[13]

Several methods have been developed to calculate the band structures of semiconductors, among them is the so-called empirical pseudo-potential method (EPM).[14−32] In the EPM 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 cancelled by the large positive kinetic energy of the electron due to its rapid oscillation.[20−26]

Temperature and pressure are experimental parameters that can be tuned in a wide range to probe the properties of condensed matter systems. The essential properties of semiconductors are their transport mechanisms that are tightly bound to their energy band gaps. Hence, knowledge of the latter and their behaviours under pressure and at various temperatures would unable us to predict overall properties of the materials of interest.[33] The investigation of the pressure and temperature dependences of the energy gaps in semiconductors has been the subject of many studies.[14−22]

In the present study, the electronic band struc-

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ture and some optoelectronic properties, such as the energy band gap, refractive index, and high frequency dielectric constant, of the considered alloy are studied. The calculated results at some high-symmetry points [L, Γ, X] of the considered ternary alloys are calculated, and compared with the experimental data for the binary alloy compounds. The calculations are performed by using the local empirical pseudo-potential method (EPM). The alloy potential is calculated in the virtual crystal approximation including the disorder effect. The effects of composition factor x ranging from 0 to 1, temperature from (0 K to 500 K), and hydrostatic pressure from (0 kbar to 120 kbar, 1 bar=10^{-5} Pa) on the electronic band structure are also studied.

2. Theory and calculations

The electronic structure of an alloy has been calculated using the empirical pseudo-potential method (EMP).[14,30] The alloy potential is calculated in the virtual crystal approximation $\boldsymbol{V}_{\rm VCA}(\boldsymbol{r})$ which is a periodic potential besides a non-periodic potential $\boldsymbol{V}_{\rm dis}(\boldsymbol{r})$ due to the compositional disorder[4,34–36]

$$\boldsymbol{V}(\boldsymbol{r})_{\rm alloy} = \boldsymbol{V}_{\rm VCA}(\boldsymbol{r}) + \boldsymbol{V}_{\rm dis}(\boldsymbol{r}). \tag{1}$$

If the considered alloy has the form $A_xB_{1-x}C$, (AC: GaAs, BC: InAs), then $\boldsymbol{V}_{\rm VCA}(\boldsymbol{r})$ and $\boldsymbol{V}_{\rm dis}(\boldsymbol{r})$ could be written as[4,34–36]

$$\boldsymbol{V}_{\rm VCA}(\boldsymbol{r}) = x\boldsymbol{V}_{\rm AC}(\boldsymbol{r}) + (1-x)\boldsymbol{V}_{\rm BC}(\boldsymbol{r}), \tag{2}$$

$$\boldsymbol{V}_{\rm dis}(\boldsymbol{r}) = -\Omega\sqrt{x(1-x)}[\boldsymbol{V}_{\rm BC}(\boldsymbol{r}) - \boldsymbol{V}_{\rm AC}(\boldsymbol{r})], \tag{3}$$

where x is the Ga concentration, Ω is treated as an adjustable parameter which simulates the disorder effect, whose value varies from one alloy to another and equals zero when the disorder effect is neglected.

The potential $\boldsymbol{V}(\boldsymbol{r})$ of the associated binary compound could be expanded in terms of reciprocal compounds vectors $\boldsymbol{G}$ as[14]

$$\boldsymbol{V}(\boldsymbol{r}) = \sum_{\boldsymbol{G}\neq\boldsymbol{G}'} a_{nk}(\boldsymbol{G}')\big[W^{\rm S}(\Delta\boldsymbol{G})\cos(\Delta\boldsymbol{G}.\boldsymbol{\tau}) + {\rm i}W^{\rm A}(\Delta\boldsymbol{G})\sin(\Delta\boldsymbol{G}.\boldsymbol{\tau})\big], \tag{4}$$

where $W^{\rm S}$ and $W^{\rm A}$ are the symmetrical and antisymmetrical form factors, respectively, $\Delta\boldsymbol{G} = |\boldsymbol{G}-\boldsymbol{G}'|$, and $\boldsymbol{\tau} = a/8(1,1,1)$ is the position vector of each atom in the unit cell with a being the lattice constant.

The energy eigenvalues of the associated binary alloys, GaAs and InAs are calculated by using the local pseudo-potential method (EPM). The energy gaps of the considered alloys are determined by arranging these eigenvalues and setting the top of the valence band to be the zero energy. The calculated energy gaps are 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), and the form factors are adjusted until the calculated energy gaps match the corresponding experimental values. Once the accurate form factors of the associated binary alloys are determined, the form factors of the ternary alloy $Ga_xIn_{1-x}As$ are calculated from

$$W^{\rm S,A}_{{\rm Ga}_x{\rm In}_{1-x}{\rm As}} = xW^{\rm S,A}_{\rm GaAs} + (1-x)W^{\rm S,A}_{\rm InAs} - \Omega\sqrt{x(1-x)}\big[W^{\rm S,A}_{\rm InAs} - W^{\rm S,A}_{\rm GaAs}\big]. \tag{5}$$

Its lattice constant is taken, according to Vegard's rule,[37] as

$$a_{{\rm Ga}_x{\rm In}_{1-x}{\rm As}} = (1-x)a_{\rm InAs} + xa_{\rm GaAs}. \tag{6}$$

The eigenvalues and the eigenvectors of the ternary alloys are found by solving the following considered matrix equation:[14]

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

or solving the secular determinant

$$\Big\|\frac{1}{2}|\boldsymbol{k}+\boldsymbol{G}'|^2 - E_{n\boldsymbol{k}}(x) + \sum_{\boldsymbol{G}\neq\boldsymbol{G}'} V(|\boldsymbol{G}-\boldsymbol{G}'|,x)\Big\| = 0. \tag{8}$$

The adjustable parameter Ω is found in the disorder part in Eq. (5) and adjusted to give good agreement with the experimental data.

Since the aim of the present work is to study the effects of temperature, T, and hydrostatic pressure, P, besides the compositional effect, x, on the electronic structure of the alloy, Eqs. (7) and (8) could be written in a general form as

$$\frac{\hbar^2}{2m}|\boldsymbol{k}+\boldsymbol{G}'|^2A_{n,\boldsymbol{k}}(\boldsymbol{G}',x,Z) + \sum_{\boldsymbol{G}\neq\boldsymbol{G}'} A_{n,\boldsymbol{k}}(\boldsymbol{G}',x,Z)V(|\boldsymbol{G}-\boldsymbol{G}'|,x,Z) = E_{n\boldsymbol{k}}(x,Z)A_{n,\boldsymbol{k}}(\boldsymbol{G}',x,Z), \tag{9}$$

$$\Big\|\frac{1}{2}|\boldsymbol{k}+\boldsymbol{G}'|^2 - E_{n\boldsymbol{k}}(x,Z) + \sum_{\boldsymbol{G}\neq\boldsymbol{G}'} V(|\boldsymbol{G}-\boldsymbol{G}'|,x,Z)\Big\| = 0, \tag{10}$$

where Z may be T or P.

To solve Eq. (10) numerically, we use the MATLAB program, in which 65×65 matrix is based on 65 bulk reciprocal lattice vectors, $\boldsymbol{G}$'s. These values cor-

respond to $|\Delta \boldsymbol{G}|^2 = 3$, 4, and 11 for the zinc-blende structure. They satisfy the condition $|\Delta \boldsymbol{G}|^2 \leq 11$, which gives non-zero pseudo-potential. The $\boldsymbol{G}$'s values (in units of $2\pi/[a(Z)]$) are listed in Ref. [14].

For each composition, x, and a certain Z, the eigenvalues and eigenvectors for the considered alloy are calculated, and the adjusting parameter Ω is varied until agreement with the experimental data is achieved.

From these calculated energy gaps, some physical properties such as the refractive index and the dielectric constant of the considered alloy can be obtained.

The refractive index is calculated using three different models that are related directly to the energy band gap $E_{\rm g}(x, Z)$.[37]

(i) The Moss formula based on the atomic model,[38] in which the refractive index is given by

$$n(x, Z) = \sqrt[4]{\frac{h}{E_{\rm g}(x, Z)}}, \tag{11}$$

where $E_{\rm g}(x, Z)$ is the energy band gap and h is a constant equal to 108 eV.[39]

(ii) The Ravindra *et al.*'s expression,[40] in which n is given by

$$n(x, Z) = \Sigma + \eta E_{\rm g}(x, Z), \tag{12}$$

with $\Sigma = 4.084$ and $\eta = -0.62$ eV^{-1}.

(iii) The empirical relation of Herve and Vandamme[41]

$$n(x, Z) = \sqrt{1 + \Big(\frac{A}{E_{\rm g}(x, Z) + B}\Big)^2}, \tag{13}$$

with $A = 13.6$ eV and $B = 3.4$ eV.

The high-frequency optical dielectric constant $\varepsilon_\infty(x, Z)$ is estimated using the relation[25]

$$\varepsilon_\infty(x, Z) = n^2(x, Z). \tag{14}$$

3. Results and discussion

3.1. Effect of Ga concentration on E_{nk} at constant temperature and hydrostatic pressure

By solving Eq. (10) for different values of composition parameter (x), the energy band gaps at $T = 0$ K and $P = 0$ kbar are obtained. Table 1 lists the adjusted symmetrical and anti-symmetrical form factors and the lattice constants of the alloy $Ga_xIn_{1-x}As$, for different x, ($0 \leq x \leq 1$).

Table 1. Adjusted symmetric and anti-symmetric form factors and lattice constants for $Ga_xIn_{1-x}As$ alloys at $T = 0$ K and $P = 0$ kbar.

x	0	0.1	0.3	0.5	0.7	0.9	1.0
Form factors (a.u)	(InAs)						(GaAs)
$W_3^{\rm S}(T)$	−0.105375	−0.106378	−0.108147	−0.111519	−0.114095	−0.117416	−0.119709
$W_8^{\rm S}(T)$	0.000100	0.000534	0.001299	0.002758	0.003872	0.005309	0.006301
$W_{11}^{\rm S}(T)$	0.023791	0.024285	0.025156	0.026816	0.028085	0.029721	0.030850
$W_3^{\rm A}$	0.022674	0.023209	0.024151	0.025947	0.027320	0.029089	0.030311
$W_4^{\rm A}(T)$	0.022494	0.022670	0.022981	0.023573	0.024025	0.024608	0.025011
$W_{11}^{\rm A}(T)$	0.004974	0.004976	0.004979	0.004986	0.004990	0.004997	0.005001
a (a.u.)	11.448000[a]	11.354117[b]	11.200625[b]	11.047134[b]	10.893642[b]	10.740150[b]	10.682600[a]

[a]Ref. [30], [b]Ref. [36].

Table 2. Direct and indirect energy band gaps for $Ga_xIn_{1-x}As$ alloys at $T = 0$ K and $P = 0$ kbar.

$Ga_xIn_{1-x}As$	T=0 K	$E_{\rm g}^L$ (P.W)	$E_{\rm g}^x$ (P.W)	$E_{\rm g}^\Gamma$ (P.W)
(InAs)		1.1064	1.3101	0.4170
		1.133[c]	1.433[c]	0.4170[c]
$Ga_{0.1}In_{0.9}As$		1.1438	1.3286	0.4894
$Ga_{0.3}In_{0.7}As$		1.1944	1.3365	0.6100
$Ga_{0.5}In_{0.5}As$		1.3818	1.4977	0.88
$Ga_{0.7}In_{0.3}As$		1.4937	1.5715	1.0721
$Ga_{0.9}In_{0.1}As$		1.6646	1.7106	1.3312
(GaAs)		1.8023	1.8388	1.5188
		1.8150[c]	1.9810[c]	1.5190[c]

[c]Ref. [42].

The calculated direct and indirect energy gaps for the considered alloy each as a function of Ga concentration at $T = 0$ K and $P = 0$ kbar are displayed in Table 2. We note that the direct and indirect energy gaps are increased by increasing the composition x. Our results for the binary compounds of the considered alloy are compared with those corresponding experimental values[42] showing that they are in good agreement with each other.

Figure 1 shows the plots of electronic structure of $Ga_xIn_{1-x}As$ versus propagation wave vector $\boldsymbol{k}$ at $T = 0$ K and $P = 0$ kbar for two different values of Ga

concentration, $x = 0.9$ (solid line) and $x = 0.3$ (dashed line). We note that the compositional disorder effect is essential for the variation of the band gap energies of the ternary semiconductor alloy $Ga_xIn_{1-x}As$. The differences between the calculated electronic energies at $x = 0.3$ and $x = 0.9$ are about 721.2 meV at Γ point, 720.2 meV at the L point, and 374.1 meV at the X point.

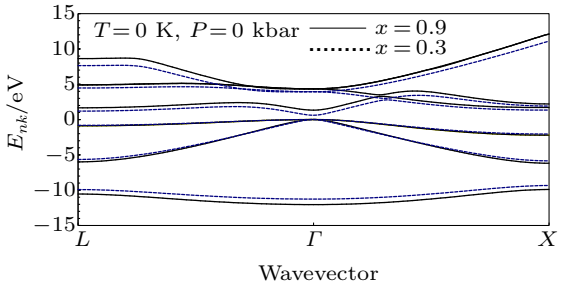


Fig. 1. (color online) The electronic structures of $Ga_xIn_{1-x}As$ at $T = 0$ K and $P = 0$ kbar for two different values of Ga concentration, $x = 0.3$ (dashed line) and $x = 0.9$ (solid line).

The dependences of the direct and indirect band gaps (E_g^Γ, E_g^L, and E_g^X) on alloy composition for $Ga_xIn_{1-x}As$ at $T = 0$ K and $P = 0$ kbar are shown in Fig. 2. We note that all the energy gaps are increased by increasing composition x. The energy gaps, E_g^Γ, E_g^L, and E_g^X increase from 0.417 eV, 1.1064 eV, and 1.3101 eV at $x = 0$ to 1.5188 eV, 1.8023 eV, and 1.8388 eV at $x = 1$, respectively. The considered alloy is a direct energy gap semiconductor in the region $0 \le x \le 1$.

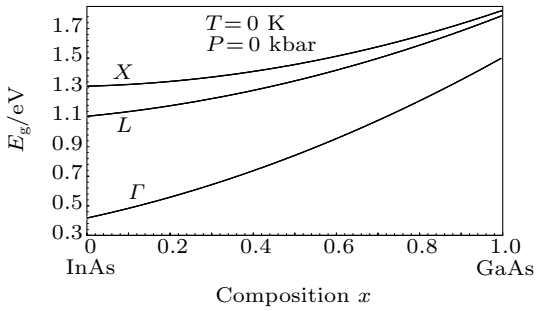


Fig. 2. Direct and indirect energy band gaps for $Ga_xIn_{1-x}As$ at $T = 0$ K and $P = 0$ kbar.

The best fittings to our results of energy gaps at $T = 0$ K and $P = 0$ kbar as functions of x yield

$$E_g^\Gamma = 0.417 + 0.6105x + 0.4773x^2, \quad (15)$$

$$E_g^X = 1.3101 + 0.0737x + 0.4406x^2, \quad (16)$$

$$E_g^L = 1.1064 + 0.2751x + 0.4082x^2. \quad (17)$$

The bowing parameters of E_g^Γ, E_g^X, and E_g^L are 0.4773 eV, 0.4406 eV, and 0.4082 eV respectively. These values of the bowing parameters are in good agreement with the published and experimental data which are found in Ref. [42].

The calculated values of the refractive index and high frequency dielectric constants, ε_∞ at $P = 0$ kbar and at $T = 300$ K are found in Table 3. We note that the refractive index and high frequency dielectric constants, ε_∞ decrease with the increase of composition x. The calculated values of the refractive index and high frequency dielectric constants, ε_∞ for the parent compounds GaAs and InAs are in sufficient agreement with the experimental values.[5,43]

Table 3. Refractive indexes and high frequency dielectric constants for $Ga_xIn_{1-x}As$ alloys at $T = 300$ K and $P = 0$ kbar.

Composition	n^L	ε_∞^L	n^X	ε_∞^X	n^Γ	$\varepsilon_\infty^\Gamma$
$x = 0$	3.1640	10.0111	3.0167	9.1003	4.1512	17.2322
(InAs)					3.51[d], 4.16[e]	12.3[d], 17.32[e]
$Ga_{0.1}In_{0.9}As$	3.1122	9.6858	2.9826	8.8960	3.8879	15.1154
$Ga_{0.3}In_{0.7}As$	3.0222	9.1336	2.9226	8.5416	3.5389	12.5236
$Ga_{0.5}In_{0.5}As$	2.9466	8.6826	2.8717	8.2466	3.3082	10.9441
$Ga_{0.7}In_{0.3}As$	2.8821	8.3067	2.8283	7.9991	3.1392	9.8546
$Ga_{0.9}In_{0.1}As$	2.8265	7.9889	2.7911	7.7905	3.0077	9.0464
$x = 1$	2.8014	7.8478	2.7746	7.6986	2.9519	8.7137
(GaAs)					3.3[d], 2.95[f]	12.9[d], 9.53[f]

[d]Ref. [43], [e]Ref. [6], [f]Ref. [5].

3.2. Effects of temperature T on E_{nk} at constant composition, x, and hydrostatic pressure P

For a given composition parameter x, and at constant pressure, $P = 0$ kbar, the temperature-dependent

eigenvalues and eigenvectors are found by solving the secular determinant to be

$$\left\| \frac{1}{2}|\boldsymbol{k}+\boldsymbol{G}'|^2 - E_{n\boldsymbol{k}}(T) + \sum_{\boldsymbol{G}\neq\boldsymbol{G}'} V(|\Delta\boldsymbol{G}|,T) \right\| = 0, \quad (18)$$

where

$$V(|\Delta\boldsymbol{G}|,T) = W^{\mathrm{S}}(\Delta\boldsymbol{G},T)\cos(\Delta\boldsymbol{G}.\boldsymbol{\tau}) + \mathrm{i}W^{\mathrm{A}}(\Delta\boldsymbol{G},T)\sin(\Delta\boldsymbol{G}.\boldsymbol{\tau}), \quad (19)$$

is the temperature-dependent empirical local pseudopotential, and $W^{\mathrm{S,A}}(\Delta\boldsymbol{G},T)$ are the symmetric, W^{S} and anti-symmetric W^{A} temperature-dependent form factors, which are fitted empirically to obtain the required energy gap for the associated binary semiconductors (GaAs gaps and InAs). The temperature-dependent form factors are calculated from the assumed relation that takes the following form:[21]

$$W^{\mathrm{S,A}}(\Delta\boldsymbol{G},T) = W^{\mathrm{S,A}}(\Delta\boldsymbol{G},T=0\ \mathrm{K}) - \Delta^{\mathrm{S,A}}T, \quad (20)$$

where $\Delta^{\mathrm{S,A}}$ is the temperature coefficient of the form factors.

The temperature-dependent lattice constant, $a(T)$ is determined from the following relation:[30]

$$a(T) = a(300\ \mathrm{K})[1+\alpha_{\mathrm{th}}(T-300\ \mathrm{K})], \quad (21)$$

where α_{th} is the linear thermal expansion coefficient. The values of α_{th} corresponding to the associated semiconductors GaAs and InAs, are listed in Table 4. The values of energy eigenvalue $E_{n\boldsymbol{k}}(T)$ are calculated at temperatures ranging from 0 to 500 K at constant x and $P = 0$ kbar, and then the direct and indirect energy gaps of the alloy compounds are determined and compared with the experimental values.

Table 4. Values of the Varshni's parameters[30] and the linear thermal expansion coefficients,[30] and the pressure coefficients[30] associated with the semiconductors used in these calculations.

Parameters	GaAs	InAs
$\alpha/10^{-4}$ K^{-2}	5.405	3.07
β/K	204	191
$\alpha_{\mathrm{th}}/10^{-6}$ K^{-1}	6.03	5
$a/10^{-2}$ eV/GPa	11.50	11.40
$b/10^{-4}$ eV/GPa^2	−24.50	0
B/GPa	75.50	57.90
B'	4.49	4.79

The experimental temperature–energy gaps are obtained from Varshni's empirical formula as[44]

$$E_{\mathrm{g}}(T) = E_{\mathrm{g}}(T=0) - \frac{\alpha T^2}{(T+\beta)}. \quad (22)$$

The values of α and β for the associated semiconductors GaAs and InAs are listed in Table 5.

Table 5. Direct and indirect energy band gaps for $Ga_xIn_{1-x}As$ alloys at $T = 300$ K, and $P = 0$ kbar.

$Ga_xIn_{1-x}As$ $T = 300$ K	E_{g}^{L}(P.W)	E_{g}^{X}(P.W)	E_{g}^{Γ}(P.W)
(InAs)	1.0776	1.3041	0.3637
	1.07[g]	1.37[g]	0.36[g]
$Ga_{0.1}In_{0.9}As$	1.1512	1.3647	0.4727
$Ga_{0.3}In_{0.7}As$	1.2946	1.4803	0.6886
$Ga_{0.5}In_{0.5}As$	1.4326	1.5881	0.9017
$Ga_{0.7}In_{0.3}As$	1.5652	1.6879	1.1121
$Ga_{0.9}In_{0.1}As$	1.6922	1.7795	1.3197
(GaAs)	1.7536	1.8222	1.4224
	1.72[h]	1.81[h]	1.42[h]

[g]Ref. [46], [h]Ref. [45].

Table 5 is similar to Table 2 but for the case at $T = 300$ K. Our results of the binary compounds of the considered alloy are compared with the corresponding experimental values,[45,46] showing that they are in very good agreement with each other.

The variations of the direct and indirect energy gaps of the considered alloy with Ga concentration at $T = 300$ K and $P = 0$ kbar are plotted in Fig. 3. The energy gaps $E_{\mathrm{g}}^{\Gamma}, E_{\mathrm{g}}^{L}$, and E_{g}^{X} increase from 0.3637, 1.0776, and 1.3041 eV at $x = 0$ to 1.4224, 1.7536, and 1.8222 eV at $x = 1$, with the increase of composition, respectively. The variation in E_{g}^{Γ} is more obvious than those in E_{g}^{L} and E_{g}^{X}. The $Ga_xIn_{1-x}As$ alloy is still a direct energy gap semiconductor at $T = 300$ K in the composition region $0 \le x \le 1$.

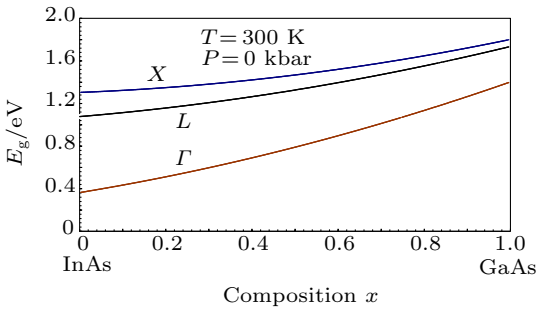


Fig. 3. (color online) Direct and indirect energy band gaps for $Ga_xIn_{1-x}As$ at $T = 300$ K, and $P = 0$ kbar.

The best fittings of our data of energy gaps as functions of x at $T = 300$ K, $P = 0$ kbar yield

$$E_{\mathrm{g}}^{\Gamma} = 0.3637 + 0.6656x + 0.3738x^2, \quad (23)$$

$$E_{\mathrm{g}}^{X} = 1.3041 + 0.1572x + 0.3405x^2, \quad (24)$$

$$E_{\mathrm{g}}^{L} = 1.0776 + 0.34x + 0.3183x^2. \quad (25)$$

The bowing parameters of E_{g}^{Γ}, E_{g}^{X}, and E_{g}^{L} are 0.3738 eV, 0.3405 eV, and 0.3183 eV, respectively.

These values of the bowing parameters are in good agreement with the published and experimental data which are found in Refs. [47] and [48].

Figure 4 displays the electronic energy spectra of the $Ga_{0.5}In_{0.5}As$ alloy at two different temperatures $T = 500$ K (solid line) and $T = 0$ K (dashed line) and constant pressure $P = 0$ kbar. It is seen that the first conduction energy band is more affected by temperature than the other bands and exhibits more enhancement at the Γ point of symmetry. The energy differences between the calculated electronic energies at $T = 0$ K and $T = 500$ K are about 156.1 meV at Γ point, 97.2 meV at the L point, and 56.9 meV at the X point. In general, the effect of temperature on energy band is small, which could be neglected.

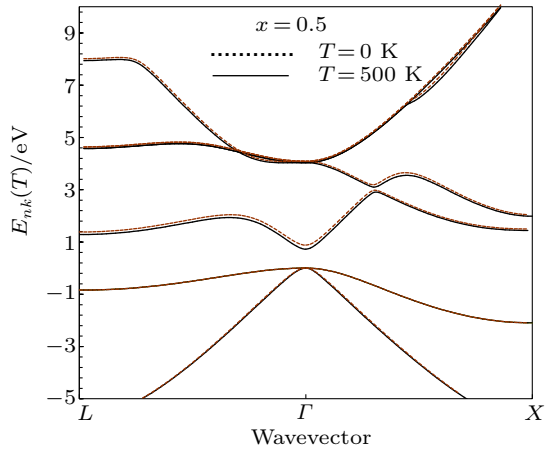


Fig. 4. (color online) Electronic energy spectra of $Ga_xIn_{1-x}As$ with $x = 0.5$ at $P = 0$ kbar and two different temperatures, $T = 0$ K (dashed line) and $T = 500$ K (solid line).

The dependences of the direct and indirect band gaps (E_g^Γ, E_g^L, and E_g^X) of the alloy $Ga_{0.5}In_{0.5}As$ at $P = 0$ kbar on temperature ranging from 0 K to 500 K are shown in Fig. 5. All energy bands decrease linearly with temperature increasing. The considered alloy is still a direct energy gap semiconductor in the temperature range $0\ \text{K} \le T \le 500$ K.

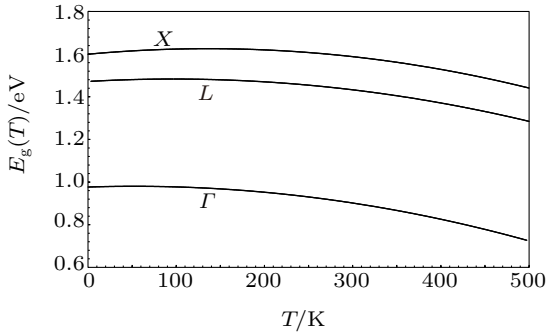


Fig. 5. Direct and indirect energy band gaps for $Ga_xIn_{1-x}As$ versus temperature at $P = 0$ kbar and $x = 0.5$.

Figure 6 shows the bowing parameters versus temperature at Γ, X, and L symmetry points. We note that the bowing parameters are slightly decreasing in the range (0 K to 300 K) from 0.4773 eV to 0.3738 eV at Γ point, 0.4082 eV to 0.3183 eV at L point, and 0.4406 eV to 0.3405 eV at X point, and then increasing from 0.3738 eV to 0.4808 eV at Γ point, 0.3183 eV to 0.4247 eV at L point, and 0.3405 eV to 0.4639 eV at X point in the region (300 K to 500 K). These results agree with the recommended assumption that the bowing parameter is independent of temperature.[42]

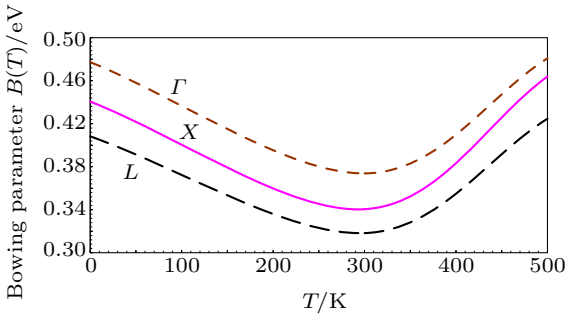


Fig. 6. (color online) Bowing parameters for $Ga_xIn_{1-x}As$ versus temperature.

The best fittings to the bowing parameter as functions of temperature give

$$B^L(T) = 0.4082 - 0.0008T + 2x10^{-6}T^2, \quad (26)$$

$$B^\Gamma(T) = 0.4773 - 0.0009T + 2x10^{-6}T^2, \quad (27)$$

$$B^X(T) = 0.4406 - 0.0009T + 2x10^{-6}T^2. \quad (28)$$

3.3. Effects of hydrostatic pressure P on E_{nk} at constant composition, x, and temperature T

For a given composition parameter x, and at constant temperature, $T = 300$ K, the pressure-dependent eigenvalues and eigenvectors are found by solving the secular determinant as follows:

$$\left\| \frac{1}{2}|\boldsymbol{k} + \boldsymbol{G}'|^2 - E_{n\boldsymbol{k}}(P) + \sum_{\boldsymbol{G}\neq\boldsymbol{G}'} V(|\Delta\boldsymbol{G}|, P) \right\| = 0, \quad (29)$$

where

$$V(|\Delta\boldsymbol{G}|, P) = W^{\mathrm{S}}(\Delta\boldsymbol{G}, P)\cos(\Delta\boldsymbol{G}.\boldsymbol{\tau}) + \mathrm{i}W^{\mathrm{A}}(\Delta\boldsymbol{G}, P)\sin(\Delta\boldsymbol{G}.\boldsymbol{\tau}) \quad (30)$$

is the pressure-dependent empirical local pseudopotential, $W^{\mathrm{S,A}}(\Delta\boldsymbol{G}, P)$ are the pressure-dependent form factors of InAs or GaAs, which are fitted empirically to the experimental values to obtain the experimental energy gaps for the associated semiconductor, which is considered to take the following form:[22]

$$W^{\mathrm{S,A}}(\Delta\boldsymbol{G}, P) = W^{\mathrm{S,A}}(\Delta\boldsymbol{G}, P = 0\ \text{kbar}) + \Delta^{\mathrm{S,A}}P, \quad (31)$$

where $\Delta^{\mathrm{S,A}}$ are the pressure coefficient form factors.

The experimental pressure-dependent energy gaps are obtained from the following empirical relation:[30]

$$E_{\mathrm{g}}^{\mathrm{d,id}}(P) = E_{\mathrm{g}}^{\mathrm{d,id}}(0) + bP + cP^2, \qquad (32)$$

where b and c are the pressure coefficients listed in Table 4, d and id denote direct and indirect energy bands respectively.

The pressure-dependent lattice constant is estimated using the following relation given by Adachi:[30]

$$a(P) = a(0)\left[1+\left(\frac{B'}{B}\right)P\right]^{-1/(3B')}, \qquad (33)$$

where B is the bulk modulus, and B' is the pressure derivative of the bulk modulus which are listed in Table 4, $a(0)$ and $a(P)$ are the lattice parameters at pressures $P = 0$ and $P \neq 0$, respectively constants.

Figure 7 shows the electronic structure of $Ga_{0.5}In_{0.5}As$ at two different pressures, $P = 0$ kbar (dashed line) and $P = 120$ kbar (solid line), and constant temperature $T = 300$ K. The energy bands are more affected by pressure effect than by temperature effect. This figure shows that the first conduction energy band is more affected by pressure than the others and exhibits more enhancement at the Γ point. The differences between the calculated electronic energies at $P = 0$ kbar and $P = 120$ kbar are about 1216.1 meV at Γ point, 501.3 meV at the L point, and 149.1 meV at the X point.

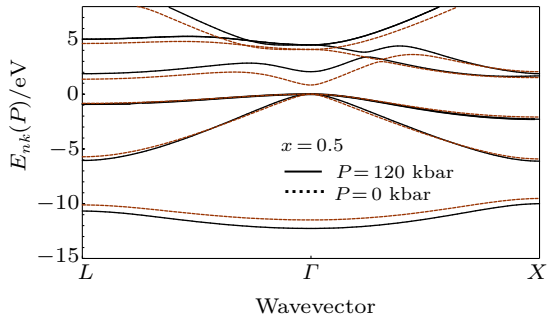


Fig. 7. (color online) Electronic structure of $Ga_xIn_{1-x}As$ with $x = 0.5$ at $T = 300$ K and two different pressures, $P = 0$ kbar (dashed line) and $P = 120$ kbar (solid line).

The dependences of the direct and indirect band gaps (E_{g}^{Γ}, E_{g}^{L}, and E_{g}^{X}) of the alloy $Ga_{0.5}In_{0.5}As$ at $T = 300$ K on pressure are shown in Fig. 8. The direct energy gap E_{g}^{Γ} and the indirect band gap E_{g}^{L} increase with pressure increasing. While the indirect band gap E_{g}^{X} slightly decreases in a range from 0 kbar to 60 kbar and slightly increases in a range from 60 kbar to 120 kbar with pressure increasing. The considered alloy has three crossover energies, the first is from L to X at nearly $P = 38$ kbar and an energy of 1.5 eV; the second is from Γ to X point at $P = 69$ kbar and an energy of 1.48 eV, and the third is from Γ to L point at $P = 90$ kbar and an energy of 1.7 eV.

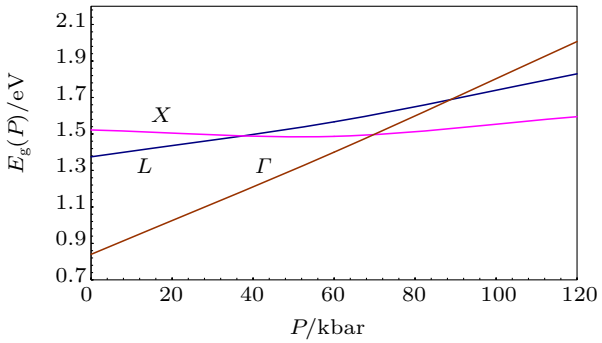


Fig. 8. (color online) Direct and indirect energy band gaps for $Ga_xIn_{1-x}As$ versus pressure at $T = 300$ K and $x = 0.5$.

Figure 9 displays the bowing parameters as functions of pressure at Γ, X, and L symmetry points. We note that the bowing parameters are very small increasing in the range (0 kbar to 60 kbar) from 0.3738 eV to 0.429 eV at Γ point, 0.3183 eV to 0.3809 eV at L point, and 0.3405 eV to 0.5012 eV at X point, but when the pressure increases from (60 kbar to 120 kbar), the bowing parameter is small decreased from 0.429 eV to 0.3231 eV at Γ point, 0.3809 eV to 0.3046 eV at L point, and 0.5012 eV to 0.0803 eV at X point.

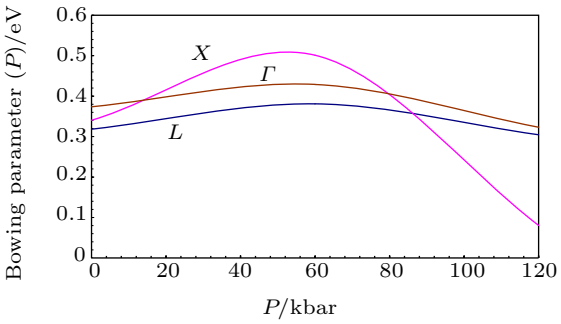


Fig. 9. (color online) Bowing parameters for $Ga_xIn_{1-x}As$ versus pressure.

The best fittings to the bowing parameter as functions of pressure give

$$B^{\Gamma}(P) = 0.3738 + 0.0023P - 2\times10^{-5}P^2, \qquad (34)$$

$$B^{X}(P) = 0.3405 + 0.0075P - 8\times10^{-5}P^2, \qquad (35)$$

$$B^{L}(P) = 0.3183 + 0.0022P - 2\times10^{-5}P^2. \qquad (36)$$

4. Conclusion

We measured the compositional, temperature and pressure dependences of the energy band gaps of $Ga_xIn_{1-x}As$ alloys in a composition range $0 \leq x \leq 1$, temperature range from 0 K to 500 K, and pressure

range from 0 kbar to 120 kbar. The calculations were performed in the virtual crystal approximation that takes into account the effect of compositional disorder. The temperature and pressure dependences of the pseudo-potential are investigated by considering temperature and pressure to be linearly dependent on pseudo-potential form factors and lattice constant. The present results show good agreements with the experimental and published data. Some of optoelectronic properties such as refractive index, dielectric constant are calculated for the considered alloy, and their variations with temperature and pressure are also studied.

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