Mechanical properties of $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system at different temperatures and pressures

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The mechanical properties, such as the elastic constants C_{11}, C_{12}, C_{44}, and bulk, Young's, and shear moduli, of a $Ga_xIn_{1-x}As_yP_{1-y}$ alloy lattice matching to a GaAs substrate are calculated for various As concentrations. The calculations are based on the pseudo-potential method within the virtual crystal approximation containing the effective disorder potential. The variations of the studied properties with pressure and temperature are investigated. A comparison between the calculated results and the available published data for binary parent compounds shows that they have good agreement, while the calculated results for the quaternary alloys at various temperature and pressure may be taken as a reference.

Keywords: elastic constants, temperature and pressure, electronic band gaps

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1. Introduction

Quaternary semiconducting materials are of continuing major concern due to their various technical applications, including light emitting diodes, lasers, optical amplifiers, detectors, frequency mixing components, and electro-optic modulators.[1] The range of device applications has been broadened in the last few decades by increasing the possibilities of engineering the material properties. The quaternary alloy $Ga_xIn_{1-x}As_yP_{1-y}$ is one of the alloys that are particularly important for manufacturing optoelectronic devices. The properties of a material under stress are determined by the elastic constants.[2] These properties have an important role in determining the binding characteristic between adjacent atomic planes, structural stability, and anisotropic characteristics of binding.[2] For the mechanical properties, a knowledge of the effect of strain on the electronic properties, specifically the elastic constants which describe the response to an applied macroscopic stress, is required.[3] Since the advent of nano-devices based on semiconductor materials, the detailed conceptions of these materials under the influence of temperature and pressure have been conveniently determined.[4]

In the present study, the elastic parameters and the relevant properties of $Ga_xIn_{1-x}As_yP_{1-y}$ quaternary alloy lattice matching GaAs substrate are investigated in a composition (y) range of 0–1, a temperature range from 0 to 500 K, and a pressure range from 0 to 120 kbar. The quaternary alloy $Ga_xIn_{1-x}As_yP_{1-y}$ is consisted as the ternary alloys $Ga_xIn_{1-x}As$, $GaAs_xP_{1-x}$, $InAs_xP_{1-x}$, and $Ga_xIn_{1-x}P$, which are bounded in their corresponding orders by four binary materials InAs, GaAs, InP, and GaP.

Our calculations are based on the empirical pseudo-potential method (EPM) within the virtual crystal approximation (VCA) including the effective disorder potential.[5–22] We also study the variations of the mechanical properties of interest for the $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system with temperatures and pressures. The calculated results for the binary parent compounds GaP, GaAs, InP, and InAs show good agreement with the available experimental and published data.

The rest of this paper is organized as follows. In Section 2, we briefly describe the calculation method. Our results and discussion are given in Section 3. And our conclusion is presented in Section 4.

2. Computational method

Initially, the energy band gaps of the binary parent compounds GaAs, GaP, InAs, and InP are calculated by using EPM. In EPM, one needs to solve the Schrödinger equation in which the one-electron pseudo-potential is represented by a linear superposition of the atomic potentials which are adjusted to fit well with the experimental values at the selected points L, Γ, and X in the Brillouin zone.

The band gap energies are estimated by numerically solving the secular determinant equation[12,13]

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

where

$$V(\left|\boldsymbol{G}-\boldsymbol{G}'\right|, Z) = W^{\mathrm{s}}(\Delta\boldsymbol{G}, Z)\cos(\Delta\boldsymbol{G}\boldsymbol{\tau}) + \mathrm{i}W^{\mathrm{a}}(\Delta\boldsymbol{G}, Z)\sin(\Delta\boldsymbol{G}\boldsymbol{\tau}) \quad (2)$$

is the Z-dependent pseudo-potential, and Z may be pressure p or temperature T.

The symmetrical W^{s} and anti-symmetrical W^{a} form factors of the parent binary compounds of $Ga_xIn_{1-x}As_yP_{1-y}$

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are deduced by fitting the calculated band gap energies to match the experimental values available in the literature. The temperature- and pressure-dependent form factors are obtained from the assumed relations[5,6]

$$W^{\mathrm{s,a}}(\Delta G, T) = W^{\mathrm{s,a}}(\Delta G, T = 0\ \mathrm{K}) - \Delta_T^{\mathrm{s,a}} T, \quad (3)$$

$$W^{\mathrm{s,a}}(\Delta G, p) = W^{\mathrm{s,a}}(\Delta G, 0) + \Delta_p^{\mathrm{s,a}} p, \quad (4)$$

where $\Delta_T^{\mathrm{s,a}}$ and $\Delta_p^{\mathrm{s,a}}$ are the temperature- and pressure-dependent coefficients of the form factors, respectively.[5,6]

The temperature- and pressure-dependent lattice constants of the binary compounds are calculated from the following relations:[21]

$$a(T) = a(300\ \mathrm{K})[1 + \alpha_{\mathrm{th}}(T - 300\ \mathrm{K})], \quad (5)$$

$$a(p) = a(0)[1 + (B'/B)p]^{-1/(3B')}, \quad (6)$$

where α_{th}, B, and B' are constants cited from Ref. [21].

The band gap energies of the parent binary compounds GaAs, InP, GaP, and InAs at different temperatures and pressures are displayed in Table 1. A comparison between our calculated data and the published ones show that they are in excellent agreement with each other. Table 2 shows the adjusted form factors of the binary materials GaAs, GaP, InP, and InAs for various temperatures and pressures.

The next step is to study the band gap energies of the associated ternary compounds, namely, $Ga_xIn_{1-x}As$, $GaAs_xP_{1-x}$, $InAs_xP_{1-x}$, and $Ga_xIn_{1-x}P_y$, and deduce their bowing parameter energies which are used to calculate the form factors of the quaternary alloy of interest,

$$\begin{aligned} & W(x,Z) \\ &= W^{\mathrm{VCA}}(x,Z) - x(1-x)[yC_{\mathrm{GaInAs}}(Z) + (1-y)C_{\mathrm{GaInP}}(Z)] \\ &\quad - y(1-y)[xC_{\mathrm{GaAsP}}(Z) + (1-x)C_{\mathrm{InAsP}}(Z)], \end{aligned} \quad (7)$$

with

$$\begin{aligned} & W^{\mathrm{VCA}}(x,Z) \\ &= xyW_{\mathrm{GaAs}}(Z) + (1-x)yW_{\mathrm{InAs}}(Z) + x(1-y)W_{\mathrm{GaP}}(Z) \\ &\quad + (1-x)(1-y)W_{\mathrm{InP}}(Z), \end{aligned} \quad (8)$$

where $C_{\mathrm{GaInAs}}(Z)$, $C_{\mathrm{GaInP}}(Z)$, $C_{\mathrm{GaAsP}}(Z)$, and $C_{\mathrm{InAsP}}(Z)$ are the Z-dependent bowing parameters of the associated ternary alloys.

Table 3 shows the bowing parameters of the considered ternary alloys $Ga_xIn_{1-x}As$, $GaAs_xP_{1-x}$, $InAs_xP_{1-x}$, and $Ga_xIn_{1-x}P_y$ at different pressures and temperatures in comparison with the available experimental values.[26–29]

The lattice constants of the quaternary $Ga_xIn_{1-x}As_yP_{1-y}$ alloys are calculated by using Vegard's rule[30]

$$\begin{aligned} a(x,Z) &= xya_{\mathrm{GaAs}}(Z) + (1-x)ya_{\mathrm{InAs}}(Z) \\ &\quad + x(1-y)a_{\mathrm{GaP}}(Z) + (1-x)(1-y)a_{\mathrm{InP}}(Z), \end{aligned} \quad (9)$$

where a_{GaAs}, a_{InAs}, a_{GaP}, and a_{InP} are the Z-dependent lattice constants of the binary compounds GaAs, InAs, GaP, and InP, respectively.

The lattice matching of $Ga_xIn_{1-x}As_yP_{1-y}$ alloy to GaAs substrate gives a relationship between the Ga and As concentrations (x and y)[14]

$$x(Z) = \frac{a_0(Z) + a_1(Z)y}{b_0(Z) + b_1(Z)y}, \quad 0 \le y \le 1, \quad (10)$$

where

$$a_0(Z) = a_{\mathrm{sub}}(Z) - a_{\mathrm{InP}}(Z), \quad (11)$$

$$a_1(Z) = a_{\mathrm{InP}}(Z) - a_{\mathrm{InAs}}(Z), \quad (12)$$

$$b_0(Z) = a_{\mathrm{GaP}}(Z) - a_{\mathrm{InP}}(Z), \quad (13)$$

$$b_1(Z) = a_{\mathrm{InP}}(Z) - a_{\mathrm{GaP}}(Z) - a_{\mathrm{InAs}}(Z) + a_{\mathrm{GaAs}}(Z), \quad (14)$$

with a's being the Z-dependent lattice constants of the binary compounds. The lattice constants of the binary compounds InAs, GaP, InP, and GaAs at different temperatures and pressures are displayed in Table 4.

Table 1. Energy band gaps at different temperature and pressure for the parent binary compounds GaAs, InAs, InP, and GaP.

Effect of temperature at $p = 0$ kba													
T/K	GaAs			GaP			InAs			InP			
	E_g^L/eV	E_g^Γ/eV	E_g^X/eV	E_g^L/eV	E_g^Γ/eV	E_g^X/eV	E_g^L/eV	E_g^Γ/eV	E_g^X/eV	E_g^L/eV	E_g^Γ/eV	E_g^X/eV	
0	1.7428	1.519	1.519[a]	1.7796	2.6988	2.7523	2.3254	2.340[d]	1.1064	0.417	0.417[d]	1.3101	1.8938	1.422	1.422[d]	2.1544
300	1.6957	1.4318	1.425[b]	1.7643	2.5959	2.5781	2.2635	2.2689[d]	1.0776	0.3637	0.3637[d]	1.3041	1.8586	1.3582	1.3582[d]	2.1444
500	1.6641	1.3735	1.3270[c]	1.7539	2.4511	2.3412	2.1618	2.1838[d]	1.0583	0.3281	0.3281[d]	1.3000	1.8164	1.2873	1.2873[d]	2.1239
Effect of pressure at $T = 300$ K													
p/kbar	GaAs			GaP			InAs			InP			
	E_g^L/eV	E_g^Γ/eV	E_g^X/eV	E_g^L/eV	E_g^Γ/eV	E_g^X/eV	E_g^L/eV	E_g^Γ/eV	E_g^X/eV	E_g^L/eV	E_g^Γ/eV	E_g^X/eV	
0	1.7375	1.4318	1.425[b]	1.7921	2.5959	2.5781	2.2635	2.2689[d]	1.0776	0.3637	0.3637[d]	1.3041	1.8532	1.3582	1.3582[d]	2.1404
30	1.9398	1.7499		1.7857	1.5051	2.4035	0.92878		1.2171	0.6973		1.2953	1.9459	1.596		2.1162
60	2.1211	2.0287		1.7808	1.5051	2.4035	0.92878		1.3739	1.0402		1.3155	2.0459	1.842		2.1082
90	2.2795	2.2636		1.7727	1.5051	2.4035	0.92878		1.5415	1.3881		1.3558	2.1509	2.088		2.1126

[a] Ref. [23], [b] Ref. [24], [c] Ref. [21], [d] Ref. [25]

Table 2. The adjusted form factors of the binary materials GaAs, GaP, InP, and InAs for various temperatures and pressures.

Effect of temperature at $p = 0$ kba												
T/K	GaAs						GaP					
	w_3^s	w_8^s	w_{11}^s	w_3^a	w_4^a	w_{11}^a	w_3^s	w_8^s	w_{11}^s	w_3^a	w_4^a	w_{11}^a
0	–0.11970	0.006301	0.030850	0.030311	0.025011	0.005001	–0.122349	0.013649	0.038835	0.045149	0.031649	0.010149
300	–0.11990	0.006299	0.029850	0.030259	0.024999	0.004999	–0.122499	0.013499	0.036999	0.044999	0.031499	0.009999
500	–0.12004	0.006298	0.029183	0.030224	0.024991	0.004998	–0.1225995	0.013399	0.034515	0.044899	0.031399	0.009899
	InAs						InP					
0	–0.105375	0.000100	0.023791	0.022674	0.022494	0.004974	–0.11490	0.005100	0.028394	0.035100	0.025100	0.005100
300	0.105399	0	0.023300	0.022599	0.022419	0.004899	–0.11500	0.005000	0.027762	0.035000	0.025000	0.005000
500	–0.105415	–0.00006	0.022973	0.022549	0.022369	0.004849	–0.11506	0.004933	0.027055	0.034933	0.024933	0.004933
Effect of pressure at $T = 300$ K												
p/kba	GaAs						GaP					
	w_3^s	w_8^s	w_{11}^s	w_3^a	w_4^a	w_{11}^a	w_3^s	w_8^s	w_{11}^s	w_3^a	w_4^a	w_{11}^a
0	–0.11990	0.006299	0.029850	0.030259	0.024999	0.004999	–0.12249	0.013499	0.036999	0.044999	0.031499	0.009999
60	–0.11409	0.007299	0.033550	0.043741	0.025999	0.005999	–0.12249	0.013509	0.041200	0.045009	0.031509	0.010009
120	–0.10827	0.008299	0.037250	0.057223	0.026999	0.006999	–0.12248	0.013519	0.044600	0.045019	0.031519	0.010019
	InAs						InP					
0	0.105399	0	0.023300	0.022599	0.022419	0.004899	–0.11500	0.005000	0.027762	0.035000	0.025000	0.005000
60	–0.105355	0.000044	0.030814	0.022643	0.022463	0.004943	–0.11473	0.005267	0.033465	0.035267	0.025267	0.005267
120	–0.105311	0.000088	0.038328	0.022687	0.022507	0.004987	–0.11446	0.005533	0.039039	0.035533	0.025533	0.005533

Table 3. Bowing parameters of the parent ternary alloys at various temperatures and pressures.

Temperature effect at $p = 0$ kbar																		
$Ga_xIn_{1-x}As$										$Ga_xIn_{1-x}P$								
$T = 0$ K			$T = 300$ K			$T = 500$ K				$T = 0$ K			$T = 300$ K			$T = 500$ K		
b^Γ	b^X	b^L	b^Γ	b^X	b^L	b^Γ	b^X	b^L		b^Γ	b^X	b^L	b^Γ	b^X	b^L	b^Γ	b^X	b^L
0.40	0.44	0.40	0.37	0.34	0.31	0.48	0.46	0.42		0.44	0.43	0.45	0.48	0.39	0.48	0.52	0.37	0.50
0.48[a]		0.33[a]	0.40[b]							0.60[a]	0.20[a]		0.60[b]	0.35[c]	0.46[c]			
$GaAs_xP_{1-x}$										$InAs_xP_{1-x}$								
0.12	0.33	0.22	0.18	0.30	0.26	0.22	0.28	0.28		0.22	0.22	0.19	0.22	0.22	0.19	0.21	0.22	0.18
0.19[a]	0.24[a]	0.16[a]	0.21[d]		0.25[d]					0.10[a]	0.27[a]	0.27[a]						
Pressure effect at $T = 300$ K																		
$Ga_xIn_{1-x}As$										$Ga_xIn_{1-x}P$								
$p = 0$ kbar			$p = 60$ kbar			$p = 120$ kbar				$p = 0$ kbar			$p = 60$ kbar			$p = 120$ kbar		
b^Γ	b^X	b^L	b^Γ	b^X	b^L	b^Γ	b^X	b^L		b^Γ	b^X	b^L	b^Γ	b^X	b^L	b^Γ	b^X	b^L
0.37 0.40[c]	0.34	0.31	0.42	0.50	0.38	0.32	0.08	0.30		0.48 0.60[b]	0.39	0.48	0.33	0.33	0.45	0.19	0.28	0.43
$GaAs_xP_{1-x}$										$InAs_xP_{1-x}$								
0.18 0.21[t]	0.30	0.26 0.25[d]	0.06	0.12	0.16	0.20	–0.48	0.28		0.22	0.22	0.19	0.19	0.20	0.17	0.15	0.19	0.14

[a] Ref. [26], [b] Ref. [28], [c] Ref. [27], [d] Ref. [29]

Table 4. Lattice constants of the binary compounds at different temperature and pressure.

Lattice constant/Å	$T = 0$ K, $p = 0$ kbar	$T = 300$ K, $p = 0$ kbar	$T = 500$ K, $p = 0$ kbar	$T = 300$ K, $p = 60$ kba	$T = 300$ K, $p = 120$ kbar
a_{InP}	5.8605	5.8686	5.8740	5.7327	5.6322
a_{GaAs}	5.6431	5.6533	5.6601	5.5267	5.4317
a_{InAs}	6.0492	6.0583	6.0644	5.8907	5.7745
a_{GaP}	5.4432	5.4508	5.4559	5.3440	5.2613

The important parameter required to calculate the elastic constants of the $Ga_xIn_{1-x}As_yP_{1-y}$ /GaAs quaternary system is its polarity, which is defined by Vogl[31] as

$$\alpha_p(x,Z) = -\frac{W_3^A(x,Z)}{W_3^S(x,Z)}, \tag{15}$$

where $W_3^S(x,Z)$ and $W_3^A(x,Z)$ are the x and Z-dependent symmetric and anti-symmetric form factors at $G(1,1,1)$, respectively.

The cubic crystal has only three elastic constants C_{11}, C_{12}, and C_{44}, so we calculate them by using the simplified

forms[32,35]

$$C_{11}(x,Z) = \frac{\sqrt{3}}{4d^5(x,Z)}\left[4.37\frac{\hbar^2}{m}(5+\lambda)(1-\alpha_{\rm p}^2(x,Z))^{3/2} - 0.60751(1-\alpha_{\rm p}^2(x,Z))^{1/2}\frac{\hbar^2}{m}\right], \quad (16)$$

$$C_{12}(x,Z) = \frac{\sqrt{3}}{4d^5(x,Z)}\left[4.37\frac{\hbar^2}{m}(3-\lambda)(1-\alpha_{\rm p}^2(x,Z))^{3/2} + 0.60751(1-\alpha_{\rm p}^2(x,Z))^{1/2}\frac{\hbar^2}{m}\right], \quad (17)$$

$$C_{44}(x,Z) = \frac{3(C_{11}(x,Z)+2C_{12}(x,Z))(C_{11}(x,Z)-C_{12}(x,Z))}{(7C_{11}(x,Z)+2C_{12}(x,Z))}, \quad (18)$$

where $d(x,Z)$ is the nearest-neighbor distance given by $d(x,Z) = \sqrt{3}a(x,Z)/4$, and λ is a dimensionless parameter which has a constant value.[32]

The knowledge of the elastic constants C_{11}, C_{12}, and C_{44} at different pressures and temperatures allows us to calculate the corresponding Young's (Y_0), shear (C_s), and bulk (B) moduli as follows:[34,35]

$$B(x,Z) = \frac{(C_{11}(x,Z)+2C_{12}(x,Z))}{3}, \quad (19)$$

$$C_s(x,Z) = \frac{(C_{11}(x,Z)-C_{12}(x,Z))}{2}, \quad (20)$$

$$Y_0(x,Z) = \frac{(C_{11}(x,Z)+2C_{12}(x,Z))(C_{11}(x,Z)-C_{12}(x,Z))}{(C_{11}(x,Z)+C_{12}(x,Z))}. \quad (21)$$

3. Results and discussion

The polarities of the $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system with different As compositions are calculated for various temperatures and pressures, and are displayed in Table 5. It can be seen that for the quaternary alloy with a certain y, the polarity decreases as the temperature increases from 0 to 500 K and increases as the pressure increases from 0 to 60 kbar, and then decreases.

Table 5. Polarities of $Ga_xIn_{1-x}As_yP_{1-y}$ alloys lattice matched to GaAs substrate at different temperature and pressure.

y	$p = 0$ kbar			$T = 300$ K		
	$T = 0$ K	$T = 300$ K	$T = 500$ K	$p = 0$ kbar	$p = 60$ kbar	$p = 120$ kbar
0	0.2963388	0.2946164	0.2934818	0.2946164	0.2987989	0.3104213
0.1	0.3001524	0.2983831	0.2972172	0.2983831	0.3102495	0.3069365
0.3	0.3032311	0.3014446	0.3002663	0.3014446	0.3325816	0.3016934
0.5	0.2992823	0.2975957	0.2964818	0.2975957	0.3534095	0.2986548
0.7	0.2873443	0.2858878	0.2849240	0.2858878	0.3717592	0.2976640
0.9	0.2667905	0.2657007	0.2649765	0.2657007	0.3866154	0.2985135
1	0.2532056	0.2523496, 0.25[a]	0.2517785	0.2523496	0.3924224	0.2995492

[a] Ref. [36]

In Table 6, we summarize the obtained elastic constants C_{11}, C_{12}, C_{44} and their relevant mechanical parameters B, C_s, Y_0 of $Ga_xIn_{1-x}As_yP_{1-y}$ alloy lattice matching GaAs substrate with different compositions. Good agreement is observed between the calculated results for the compositions ($x = 1$, $y = 1$) and the published data at $T = 300$ K, $p = 0$ kbar. $GaxIn_{1-x}As_yP_{1-y}$ is a very important alloy, which is actually employed in commercial optoelectronic devices, especially semiconductor lasers and in electronic devices, especially high-electron mobility transistors.[1] No experimental data are found for the polarities of other alloys. Consequently, our results may serve as a reference for future experimental work.

Table 7 shows the calculated C_{11}, C_{12}, C_{44}, B, C_s, and Y_0 for the $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system at different temperatures and pressures. It should be noted that all of the parameters slightly decrease with increasing temperature and increase with increasing pressure.

Figure 1 shows the thermal effect on the elastic constants C_{11}, C_{12}, and C_{44} for the $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system with $y = 0.5$ at $p = 0$ kbar. They decrease linearly with increasing temperature; however, C_{11} has a higher value than C_{12} and C_{44}, which are nearly constant.

Table 6. Elastic constants, bulk, shear, and Young's moduli of $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system with different y at $T = 300$ K, $p = 0$ kbar.

y	x	$C_{11}/10^{11}$ dyne·cm^{-2}	$C_{12}/10^{11}$ dyne·cm^{-2}	$C_{44}/10^{11}$ dyne·cm^{-2}	$B/10^{11}$ dyne·cm^{-2}	$C_s/10^{11}$ dyne·cm^{-2}	$Y/10^{11}$ dyne·cm^{-2}
0	0.51	12.825	5.5432	5.1791	7.9706	3.641e	9.4796
0.1	0.56	12.777	5.5236	5.1591	7.9414	3.6267	9.4426
0.3	0.65	12.737	5.5073	5.1426	7.9172	3.6148	9.4121
0.5	0.75	12.786	5.5272	5.1628	7.9468	3.6294	9.4496
0.7	0.85	12.932	5.5867	5.2234	8.0353	3.6728	9.5616
0.9	0.95	13.173	5.6843	5.3227	8.1804	3.7441	9.7455
1	1	13.322 13.32[a]	5.7453 5.74[a]	5.3847 5.29[b]	8.271 7.9[c]	3.7886 3.25[d]	9.8602 8.53[e]

[a] Ref. [37], [b] Ref. [35], [c] Ref. [38], [d] Ref. [39], [e] Ref. [21]

Table 7. Elastic constants, bulk, shear, and Young's moduli of $Ga_xIn_{1-x}As_yP_{1-y}$ with $y = 0.5$ at different temperature and pressure.

	$C_{11}/10^{11}$ dyne·cm^{-2}	$C_{12}/10^{11}$ dyne·cm^{-2}	$C_{44}/10^{11}$ dyne·cm^{-2}	$B/10^{11}$ dyne·cm^{-2}	$S/10^{11}$ dyne·cm^{-2}	$Y/10^{11}$ dyne·cm^{-2}
Effect of temperature at $p = 0$ kbar						
0	12.879	5.5683	5.2005	8.0055	3.6558	9.5184
300	12.786	5.5272	5.1628	7.9468	3.6294	9.4496
500	12.723	5.4998	5.1377	7.9076	3.6118	9.4037
Effect of pressure at $T = 300$ K						
0	12.786	5.5272	5.1628	7.9468	3.6294	9.4496
60	13.45	5.83	5.42	8.37	3.81	9.92
120	15.59	6.74	6.29	9.69	4.42	11.52

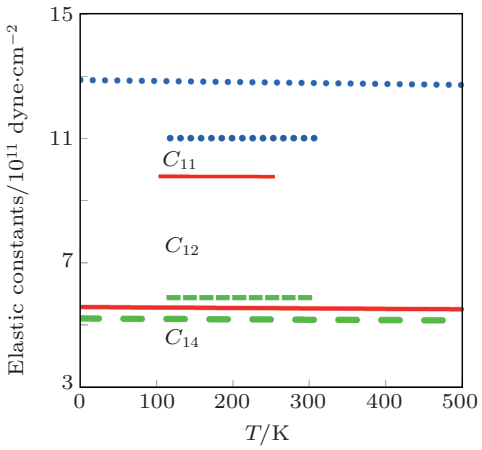


Fig. 1. (color online) Elastic constants of $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system at $p = 0$ kbar.

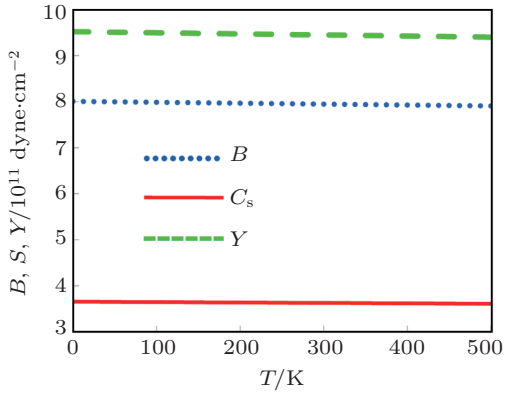


Fig. 2. (color online) Bulk, shear, and Young's moduli of $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system at $p = 0$ kbar.

The temperature dependences of shear, Young's, and bulk moduli of the $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system with $y = 0.5$ at $p = 0$ kbar are investigated and displayed in Fig. 2. All of the parameters slowly decrease with increasing temperature.

Figure 3 shows the pressure dependences of the elastic constants C_{11}, C_{12}, and C_{44} of the $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system with $y = 0.5$ at $T = 300$ K. The elastic constants C_{11}, C_{12}, and C_{44} increase as pressure increases from 0 to 120 kbar, and the increase of C_{11} is larger than that of C_{12} and C_{44}.

Figure 4 shows the variations of B, C_s, and Y_0 with pressure for the Ga_xIn_{1-x} As_yP_{1-y}/GaAs system with $y = 0.5$ at $T = 300$ K. As can be seen from the figure, the variations of these parameters with pressure are small. They increase as pressure increases from 0 to 120 kbar. All of the parameters slowly increase with increasing pressure over the whole region of 0–120 kbar.

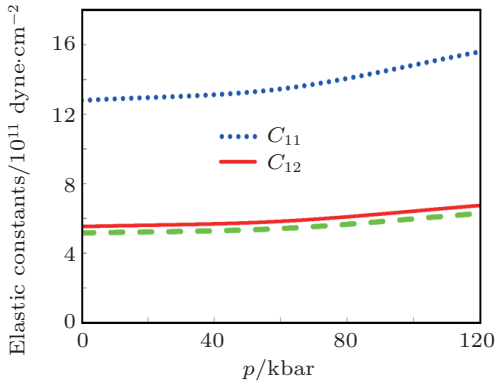


Fig. 3. (color online) Elastic constants of $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system at $T = 300$ K.

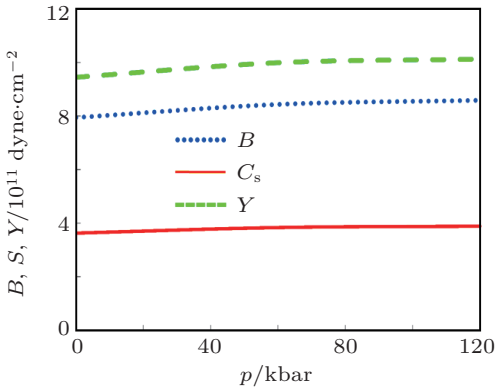


Fig. 4. (color online) Bulk, shear, and Young's moduli of $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system at $T = 300$ K.

4. Conclusion

The polarities of the quaternary alloys $Ga_xIn_{1-x}As_yP_{1-y}$ lattice matching GaAs substrate are calculated with various compositions y at different temperatures and pressures. The elastic constants C_{11}, C_{12}, and C_{44} and the corresponding mechanical properties, such as bulk, shear, and Young's moduli, of the $Ga_xIn_{1-x}As_yP_{1-y}$/GaAs system are investigated. The variations of all of the properties of interest under the influence of temperature and pressure are investigated. A comparison between our calculated results and the available experiment and published data for the binary parent compounds

shows that they have a very good agreement, while the calculated results for the quaternary alloys at various temperatures and pressures may be taken as a reference.

References

[1] Vurgaftman I, Meyer J R and Ram-Mohan L R 2001 *J. Appl. Phys.* **89** 5815
[2] Ghebouli M A, Ghebouli B and Fatmi M 2011 *Physica B* **406** 1837
[3] Ghebouli B, Ghebouli M A and Fatmi M 2011 *Physica B* **406** 2521
[4] Shimomura H, Anan T and Sugou S 1996 *J. Cryst. Growth* **162** 121
[5] Elabsy A M and Elkenany E B 2010 *Physica B* **405** 266
[6] Elabsy A M, Degheidy A R, Abdelwahed H G and Elkenany E B 2010 *Physica B* **405** 3709
[7] Degheidy A R and Elkenany E B 2011 *Semiconductors* **45** 10
[8] Elabsy A M 2011 *Advances in Condensed Matter and Material Research* **75**
[9] Degheidy A R, Elabsy A M, Abdelwahed H G and Elkenany E B 2012 *Indian J. Phys.* **86** 363
[10] Degheidy A R and Elkenany E B 2012 *The African Review of Physics* **7** 0014
[11] Degheidy A R, Elabsy A M and Elkenany E B 2012 *Superlattices and Microstructures* **52** 336
[12] Degheidy A R and Elkenany E B 2012 *Mat. Sci in Semiconductor Processing* **15** 505
[13] Degheidy A R and Elkenany E B 2012 *Chin. Phys. B* **21** 12
[14] Degheidy A R and Elkenany E B 2013 *Materials Chemistry and Physics* **143** 1
[15] Degheidy A R and Elkenany E B 2013 *Semiconductors* **47** 1283
[16] Degheidy A R, Sayed A and Elkenany E B 2013 *J. Alloy. Compd.* **574** 580
[17] Degheidy A R and Elkenany E B 2013 *Thin Solid Films* **539** 365
[18] Degheidy A R and Elkenany E B 2011 *Proceedings of the 8th Conference on Nuclear and Particle Physics,* November 20–24, 2011 Hurghada, Egypt
[19] Samara G A 1983 *Phys. Rev. B* **27** 3494
[20] Welber B, Cardona M, Kim C K and Rodriguez S 1975 *Phys. Rev. B* **12** 5729
[21] Adachi S 2005 *Properties of Group-IV, III–V and II–VI Semiconductors* (New York: Wiley)
[22] Peter Y U and Cardona M 2010 *Fundamentals of Semiconductors* (4th Edn.) (Berlin: Springer)
[23] Piprek J 2003 *Semiconductor Optoelectronic Devices* (New York: Academic Press)
[24] Lee H J, Juravel L V and Woolley J C 1980 *Phys. Rev. B* **21** 659
[25] Varshni Y P 1967 *Physica* **34** 149
[26] Adachi S 1992 *Physical Properties of III–V Semiconductor Compounds: InP, InAs,GaAs, GaP, InGaAs, and InGaAsP* (New York: Wiley)
[27] Boucenna M and Bouarissa N 2004 *Mater. Chem. Phys.* **84** 375
[28] Muller H, Trommer R, Cardona M and Vogl P 1980 *Phys. Rev. B* **21** 4879
[29] Vurgaftman I, Meyer J R and Ram-Mohan L R 2001 *J. Appl. Phys.* **89** 5815
[30] Vegard L Z 1921 *Physics* **5** 17
[31] Vogl P 1978 *J. Phys. C* **11** 251
[32] Baranowski J M 1984 *J. Phys. C* **17** 6287
[33] Bouarissa N 2003 *Materials Science and Engineering B* **100** 280
[34] Harrison W A 1980 *Electronic Structure and the Properties of Solids* (New York: Freeman)
[35] Shen S G 1994 *J. Phys.: Condens. Matter* **6** 8733
[36] Bouarissa N and Kassali K 2004 *Superlattices and Microstructures* **35** 115
[37] Bouarissa N and Bachiri R 2002 *Physica B* **322** 193
[38] Saib S and Bouarissa N 2006 *Solid State Electron.* **50** 763
[39] Levinshtein M, Rumyantsev S and Shur M 1999 *Handbook Series on Semiconductor Parameters* **2** (Singapore: World Scientific)