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Impact of pressure and composition on the mechanical behavior of $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ quaternary alloys

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ABSTRACT

Property of matter of the semiconductors quaternary was investigated by the density functional theory and paralleled to the foretelling of the linear elasticity theory. In addition, quaternary alloys of $In_xGa_{1-x}As_{1-y}P_y$ lattice matching GaAs substrate and $Al_xIn_{1-x}Sb_{1-y}P_y$ lattice matching InSb substrate for x and y = (0, 0.25, 0.50, 0.75, and 1) compositions were studied. The elastic constants C_{11}, C_{12}, C_{44}, and bulk, Young's, and shear modulus are also calculated. Meanwhile, the results were analyzed data in different pressure. The comparison between the calculated results and the available published data for quaternary alloys displayed that they had worthy accordance at pressure p = 0 and the results at P > 0 may be required as an acceptable reference.

Introduction

The ability of Semiconductor quaternary alloys led them to being taken into consideration in order to familiarize the optoelectronic properties with progress of new semiconductor technologies, for instance, the forbidden energy and elastic constant with the alloy compositions. Overall, the technical significance of the group (Al, In, Ga, As, Sb, P) has enhanced the study of their quaternary alloys $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ especially for optoelectronic devices. It can be scrutinized as one of the central ingredients for the manufacture of optoelectronic devices including the surface emitting long wavelength semiconductor lasers [1]. The recent study of the quaternary alloys has been emphasized. Material engineering can get more opportunities through Quaternary alloys containing controlling the energy band gap and the lattice constant within definite limitations. Thus, the significance of fabrication procedure roles effectively in optoelectronic engineering [2]. Remarkable recent research has emphasized on the structural stability of some quaternary alloys in diverse pressure, but they did not clearly mention the high-pressure phase diagrams of the $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ quaternary alloys. It reasonably led to certain sample-handling difficulties that occurred in dealing with these alloys. Experientially, all of the alloys take on the zinc-blende structure at low and moderate pressure. A study has been already conducted on $In_xGa_{1-x}As_{1-y}P_y$ structure and optical properties using density functional theory [3], but then another study has been directed to simulated elastic parameters of the ternary alloys with effect pressure [4]. Besides, a variety of studies theoretically and experimentally referred to the structure and other physical properties of some quaternary alloys [5–7].

In this work, mechanical performers of $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ quaternary semiconductor alloys for x and y compositions at a constant temperature under different pressure have been newly indicated. The existent study was done in order to illuminate the studies which will be practically created, to assist them in determining the change in amounts of additives in alloys. Mechanical characteristic of quaternary alloys differ under various pressures, which directly influence distinct applications of GaAs and InSb substrates devices under methods of other works.

Theoretical method

In this database, we are using the CASTEP program [8]. The calculation is perfected using Kohn–Sam formation [9], which used density function theory (DFT) to generalized gradient approximation (GGA) that is comprised of electronic exchange correlation potential energy, using pseudo-potential concept. A cubic unit cell is based with atoms (Ga/In) and (As/P) of $In_xGa_{1-x}As_{1-y}P_y$ alloys and founded with atoms (Al/In) and (Sb/P) of $Al_xIn_{1-x}Sb_{1-y}P_y$ quaternary alloys. After we have considered quaternary alloys as having cubic symmetry in our calculation for all the five systems to maintain uniformity and

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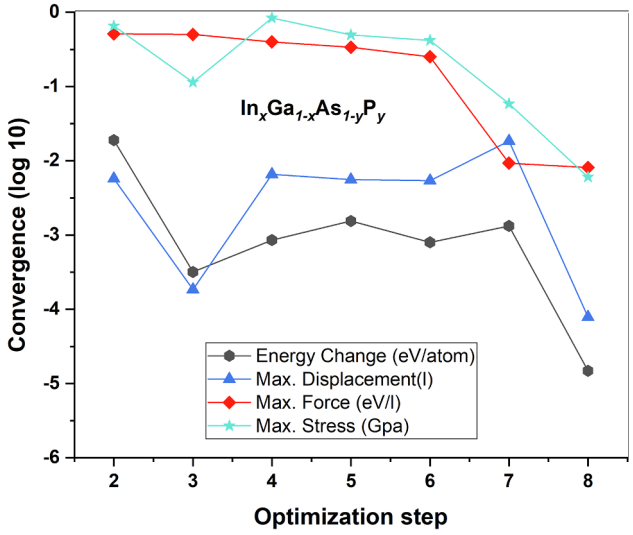

Fig. 1. The optimization step convergence of $In_xGa_{1-x}As_{1-y}P_y$ for x and y = 0.75.

simplicity. We have taken cubic unit cell for x and y we have replaced atoms, respectively to get the coveted concentrations The wave functions are widened in the plane waves up to a kinetic- energy cutoff of 880 eV. The first step of Geometry Optimization has been completed for $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys for x and y compositions at constant temperature with symmetry P1. Fig. 1 shows the diagram of the step optimization graph given only for x and y = 0.75 to save space in journal. Atomic positions are optimized with a density mixing scheme [10] using the conjugate-gradient (CG) method [11] for values minimization. The Monk-horst-Pack scheme [12] with regular integration points are applied under various pressures. The second step of the present work is to calculate the parameters of elasticity of the related $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys. Below is the internal stress and strain tensor equations used in the simulation [13]

$$\sigma = \frac{1}{k_0}\left\{\sum_{i=1}^{N} x_i(f_i f_i^T) + (\Sigma_{i>j} r_{ij} v_{ij}^T)\right. \tag{1}$$

$$\varepsilon = \frac{1}{2}[(p_0^T)^{-1} D p_0^{-1} - 1] \tag{2}$$

where

σ: stress tensor
ε: strain sensor
index i: works overall particles 1 through *N*, x_i, *fi* and v_i denote the force, velocity and mass expressible on particle *i*
k_o: the system volume.
p_0: the matrix formed from the three column vectors a_0, b_0, c_0, *p* the identical matrix formed from *a*, *b*, *c*, *T* the matrix change.
D: the metric tensor.

The elastic mixture coefficients, relating the different factors of tensors are explained by:

$$C_{lmnk} = \frac{\partial \sigma_{lm}}{\partial \sigma_{nk}}\left|\frac{1}{V_0}\frac{\partial^2 T}{\partial \varepsilon_{lm}\partial \varepsilon_{nk}}\right|_{T,\varepsilon_{lm}\varepsilon_{nk}} \tag{3}$$

where *T* the Helmholtz free energy.

$$\sigma_{lm} = C_{lmnk}\,\varepsilon_{nk} \tag{4}$$

$$\varepsilon_{lm} = S_{lmnk}\,\sigma_{nk} \tag{5}$$

These equations correlation between the stresses and strains, where S_{lmnk} the submission components,

Table 1
Lattice parameters a (A°) and band gap energy E_g (eV) of the $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys under different pressure P (kbar).

Concentrations *x* and *y*	Parameters	Present work		
		P = 0 kbar	P = 60 kbar	P = 100 kbar
$In_xGa_{1-x}As_{1-y}P_y$				
0	a (A°)	5.687	5.513	5.302
	E_g (eV)	1.339	1.624	1.963
0.25	a (A°)	5.775	5.594	5.414
	E_g (eV)	1.281	1.372	1.825
0.50	a (A°)	5.896	5.647	5.537
	E_g (eV)	1.190	1.375	1.595
0.75	a (A°)	5.923	5.663	5.473
	E_g (eV)	1.167	1.421	1.646
1	a (A°)	5.819	5.762	5.595
	E_g (eV)	1.073	1.690	2.041
$Al_xIn_{1-x}P_ySb_{1-y}$				
0	a (A°)	6.443	6.215	5.931
	E_g (eV)	0.682	1.195	1.818
0.25	a (A°)	6.051	5.907	5.857
	E_g (eV)	0.894	0.919	0.960
0.50	a (A°)	5.848	5.801	5.796
	E_g (eV)	1.734	1.792	2.269
0.75	a (A°)	5.813	5.772	5.650
	E_g (eV)	1.997	2.017	2.631
1	a (A°)	5.501	5.452	5.328
	E_g (eV)	3.478	3.512	3.645

Table 2
Elastic constant moduli of the $In_xGa_{1-x}As_{1-y}P_y$ alloys under different pressure.

x, *y*	Pressure (kbar)	$C_{11} \times 10^{11}$ (dyne.cm^2)	$C_{12} \times 10^{11}$ (dyne.cm^2)	$C_{44} \times 10^{11}$ (dyne.cm^2)
0	0	12.671	5.631	5.438
	60	13.061	5.982	6.317
	100	13.173	7.192	6.692
0.25	0	12.717	5.472	5.993
	60	13.041	6.037	6.310
	100	13.292	6.903	7.121
0.50	0	12.813	5.504	5.930
	60	13.309	6.193	6.541
	100	14.077	6.907	7.984
0.75	0	12.938	5.502	6.127
	60	13.359	6.223	6.692
	100	14.167	7.827	7.748
1	0	13.415	5.358	6.765
	60	14.062	6.281	7.292
	100	14.968	6.915	7.835

Note that in both Eqs. (4) and (5), For example, s_{12} is given in:

$$\sigma_{12} = C_{1222}\varepsilon_{11} + C_{1221}\varepsilon_{12} + C_{1223}\varepsilon_{13} + C_{1212}\varepsilon_{21} + C_{12211}\varepsilon_{22} + C_{1213}\varepsilon_{32} + C_{1232}\varepsilon_{31} + C_{1231}\varepsilon_{32} + C_{1233}\varepsilon_{33}$$

the generalized written as:

$$\sigma_i = C_{ij}\varepsilon_j \tag{6}$$

Processes used for the bulk modulus B_u, young modulus Y_o *and* Shear modulus S_h are given as follows:

$$B_u = l + \frac{2}{3}w \tag{7}$$

$$Y_0 = w\left(\frac{3l + 2w}{l + w}\right), \quad S_h = w \tag{8}$$

where *l* and *w* are indicate to as the Lamé coefficients.

The Mechanical parameters were calculated by the limited strain process various pressure at constant temperature. In this process, the

Table 3
Elastic constant modulus of the $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys under pressure.

x, y	Pressure (kbar)	C_{11} (dyne.cm^2 × 10^{11})	C_{12} (dyne.cm^2 × 10^{11})	C_{44} (dyne.cm^2 × 10^{11})
0	0	6.673	2.854	3.042
	60	6.821	2.914	3.105
	100	7.182	2.994	3.127
0.25	0	8.076	3.162	4.193
	60	8.407	3.494	4.370
	100	8.843	3.978	4.864
0.50	0	8.939	3.992	4.312
	60	8.453	3.471	4.359
	100	8.980	4.426	4.378
0.75	0	9.362	4.115	4.341
	60	9.646	4.301	4.778
	100	10.211	4.576	5.045
1	0	13.174	5.184	5.991
	60	13.836	5.990	6.217
	100	14.017	6.430	6.528

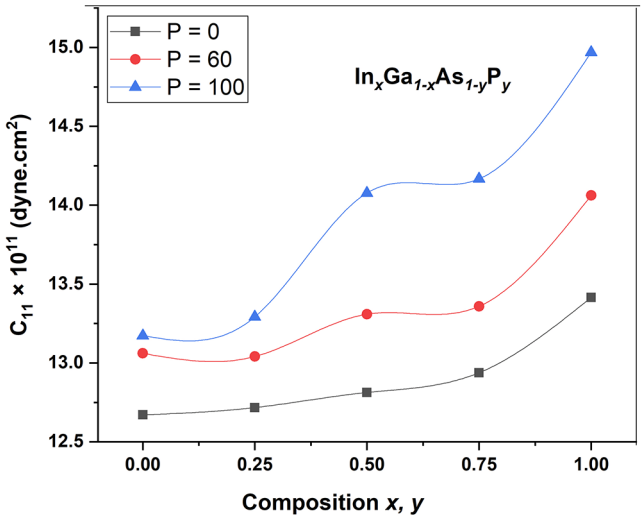

Fig. 2. Elastic constants C_{11} of $In_xGa_{1-x}As_{1-y}P_y$ alloys.

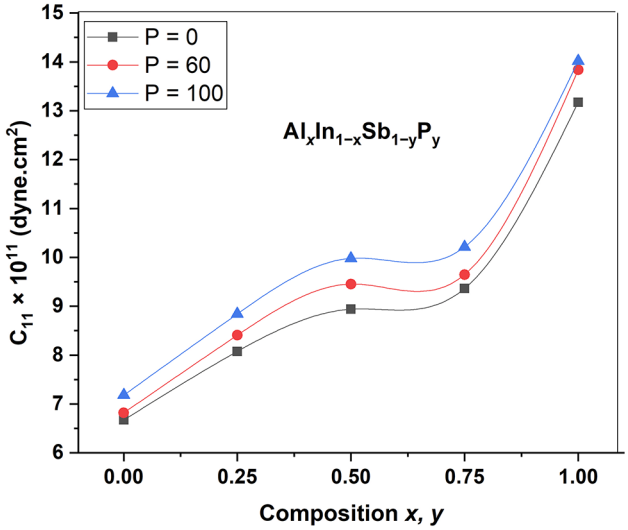

Fig. 3. Elastic constants C_{11} of $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys.

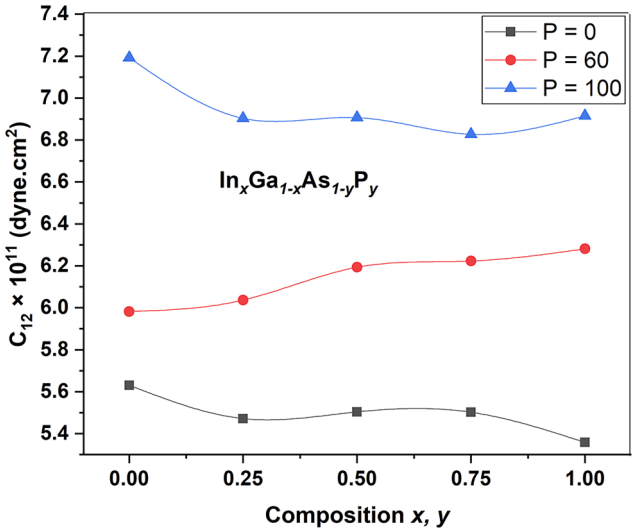

Fig. 4. Elastic constants C_{12} of $In_xGa_{1-x}As_{1-y}P_y$ alloys.

basis state structure is strained according to symmetry-dependent strain patterns with varying capacities and a subsequent calculation all parameters after are the optimization. Furthermore, the bulk modulus B_u and the shear modulus S_h were calculated from the elastic parameters. Young's modulus Y_0 was then computed from these values.

Results and discussion

The calculation was the estimation of the lattice constants of the quaternary alloys by decreasing these parameters of the crystal structure under different pressure. Besides to these lattice parameters, the calculation of the electronic energy band gap conforming to high symmetry points was done. The achieved value of the lattice constants of $In_xGa_{1-x}As_{1-y}P_y$ alloys is 1% greater than the theoretical values for pressure equal to zero [14,15]. Additionally, the lattice constants of $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys are 0.9% less than the other theoretical values [16–18].

Table 1 displays the results of lattice parameters and forbidden energy for × and y compositions under different pressure (P = 0, 60 and 100). While lattice constant decreases, forbidden energy increases with pressure increase. Elastic modulus of $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ quaternary alloys under different pressures were indicated in Tables 2 and 3. More specifically, they clarified he stability and rigidity of materials and their DFT calculation necessities in certain

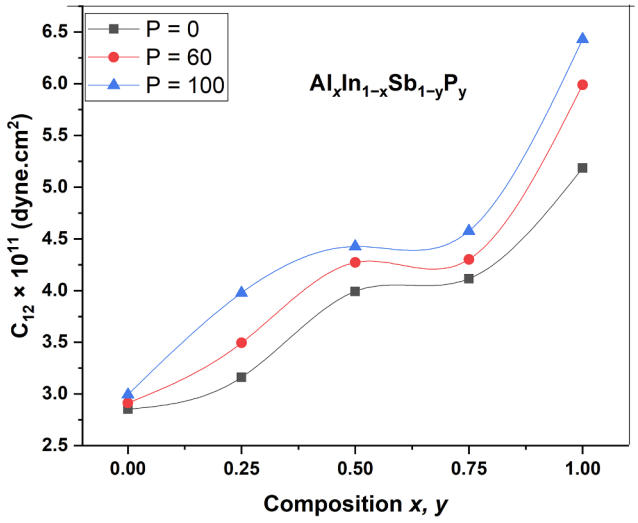

Fig. 5. Elastic constants C_{12} of $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys.

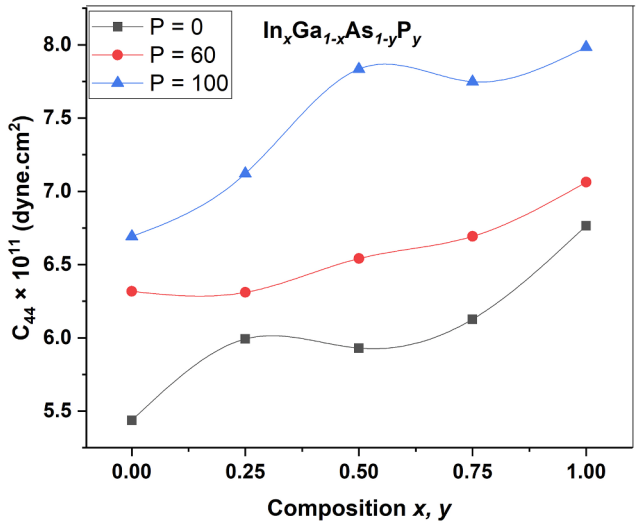

Fig. 6. Elastic constants C_{44} of $In_xGa_{1-x}As_{1-y}P_y$ alloys.

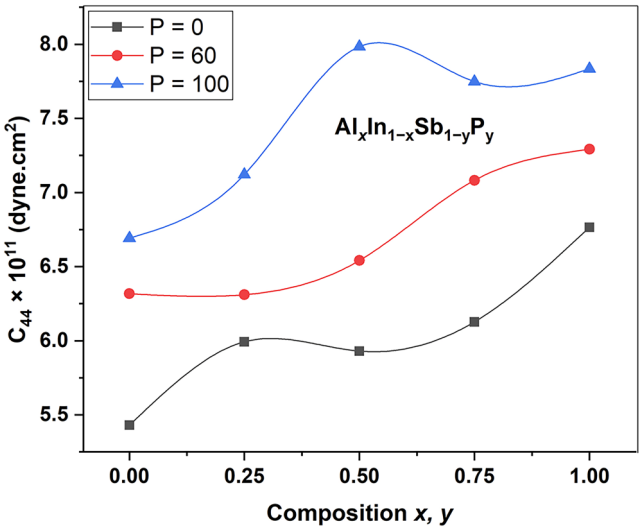

Fig. 7. Elastic constants C_{44} of $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys.

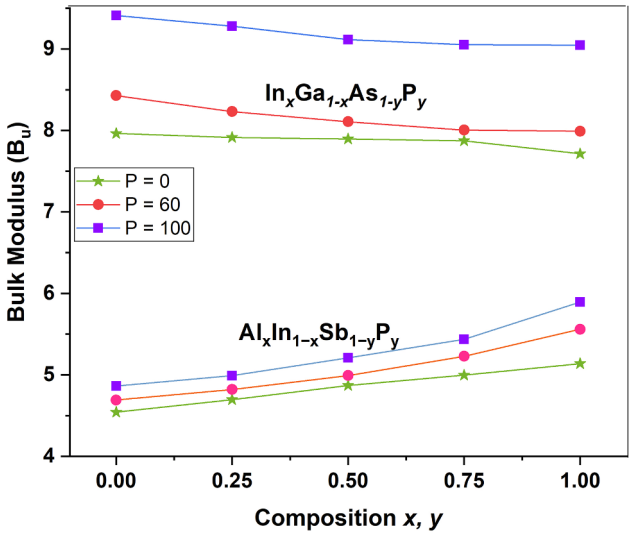

Fig. 8. Bulk modulus of $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys.

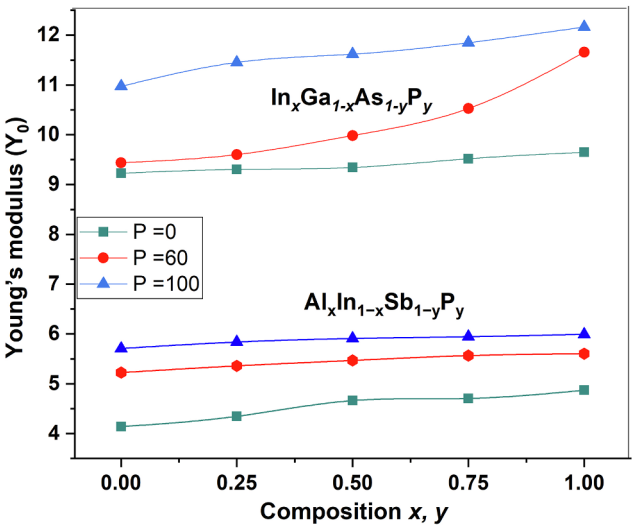

Fig. 9. Young modulus of $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys.

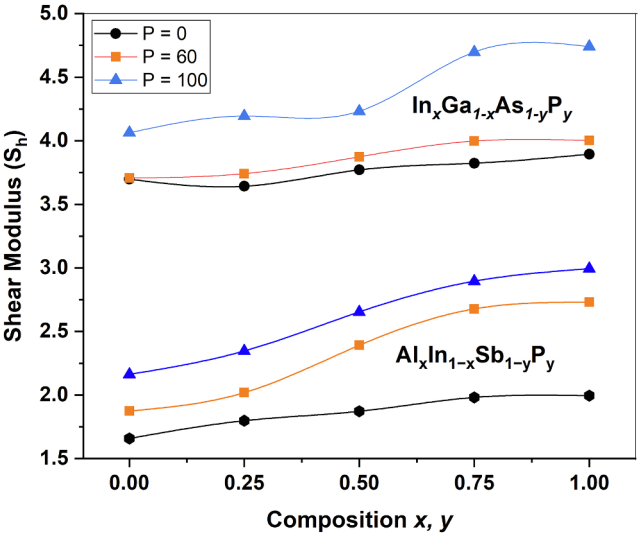

Fig. 10. Shear modulus of $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys.

Table 4
The calculated Bulk Modulus (B_u), Shear modulus (S_h) Young's modulus (Y_0) under different pressure (P) of the $In_xGa_{1-x}As_{1-y}P_y$ alloys.

x, y	B_u (dyne.cm^2 × 10^{11})			S_h (dyne.cm^2 × 10^{11})			Y_0 (dyne.cm^2 × 10^{11})		
	P = 0	P = 60	P = 100	P = 0	P = 60	P = 100	P = 0	P = 60	P = 100
0	7.962	8.427	9.410	3.698	3.780	4.063	9.227	9.440	10.973
0.25	7.914	8.232	9.279	3.642	3.541	4.195	9.304	9.601	11.453
0.50	7.895	8.107	9.116	3.701	3.674	4.232	9.343	9.984	11.618
0.75	7.874	8.004	9.052	3.723	3.699	4.898	9.519	10.526	11.847
1	8.013	7.991	9.045	3.795	4.006	4.941	9.648	11.657	12.165

Table 5
The calculated Bulk Modulus (B_u), Shear modulus (S_h) Young's modulus (Y_0) under different pressure (P) of the $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys.

x, y	B_u (dyne.cm^2 × 10^{11})			S_h (dyne.cm^2 × 10^{11})			Y_0 (dyne.cm^2 × 10^{11})		
	P = 0	P = 60	P = 100	P = 0	P = 60	P = 100	P = 0	P = 60	P = 100
0	4.541	4.691	4.863	1.658	1.874	2.163	4.138	5.225	5.708
0.25	4.696	4.820	4.992	1.798	2.019	2.347	4.346	5.358	5.839
0.50	4.870	4.992	5.210	1.872	2.391	2.654	4.662	5.469	5.910
0.75	4.996	5.228	5.436	1.981	2.678	2.895	4.704	5.566	5.946
1	5.138	5.560	5.893	1.995	2.730	2.993	4.871	5.103	5.993

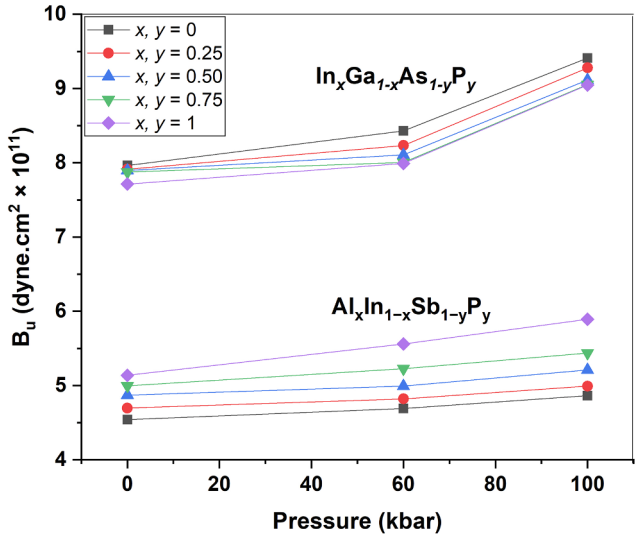

Fig. 11. Bulk modulus of the various pressures of $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ alloys.

methods.

The elastic parameters are functions and features of the first and second order derivatives of the potentials. The second-order elastic constants (Cij) for a stable cubic crystals structure is the three dependent elastic constants C_{ij} (C_{11}, C_{12}, C_{14}). They satisfy with the calculation below:

C_{11} (p) > 0, C_{44} (p) > 0, ($C_{11}-C_{12}$) (p) > 0, (C_{11} + 2C_{12}) (p) >

The results of Tables 2 and 3 about elastic constants adapt the stable conditions of various pressure values (P = 0, 60 and 100) kbar for all alloys. All of the studied about the elastic constants (C_{11}, C_{12}, C_{14}) of quaternary alloys for x and y compositions under different pressures are shown in Figs. 2–7. It explained that the elastic parameters of alloys increase with x and y compositions. In the same time, the increasing of pressure makes an increase in parameters in the alloys. As pressure increases from 0 to 100 kbar, the elastic constants increase. Nevertheless, the increasing rate of C_{11} is higher than those of C_{12} and C_{44} in all alloys.

The Figs. 8–10 point out the variations of bulk (B_u), Young (Y_0) and shear (S_h) modulus with increasing pressure for the $In_xGa_{1-x}As_{1-y}P_y$ and $Al_xIn_{1-x}Sb_{1-y}P_y$ quaternary alloys for x and *y* compositions, the figures consider that the changes in these values with x and y compositions and pressure are shown in (Tables 4 and 5).

As a result, all parameters gradually increase with pressure increasing. It demonstrated that the variations Bo with pressure of $In_xGa_{1-x}As_{1-y}P_y$ alloys were higher than $Al_xIn_{1-x}Sb_{1-y}P_y$ quaternary alloys, as seen in Fig. 11. This result is considered as a principal reference for the following works.

Conclusion

The computational method was utilized to find out the symmetrical and mechanical behavior of the semiconductors quaternary alloys of $In_xGa_{1-x}As_{1-y}P_y$ lattice matching GaAs substrate and $Al_xIn_{1-x}Sb_{1-y}P_y$ lattice matching InSb substrate for x and y compositions. Also, the alloys were being calculated under pressure (P = 0, 60 and 100 kbar) via DFT calculations. The calculation was done for Mechanical properties as the elastic constants and for their related elastic parameters bulk (B_u), Young (Y_0) and shear (S_h) modulus. The current calculated results are in common with the existent theoretical published data at P = 0 kbar. Most of our data including P = 60 and 100 kbar could be taken into consideration for other works in future.

Acknowledgements

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