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ORIGINAL PAPER

Pressure Dependence of Mechanical Properties in AlP and AlSb Semiconductors

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Abstract
The effect of pressure on the mechanical properties of zinc-blende AlP and AlSb semiconductors has been investigated using the local empirical pseudo-potential method (EPM). The studied quantities are the elastic constants(c_{ij}), bulk modulus (B_u), shear modulus (S_h),Young modulus (Y_0), Poisson's ratio (σ, bond stretching (α, bond binding force (β, internal strain parameter (ζ, linear compressibility (C_0) and Cauchy ratio (C_a). All studied quantities are found to be affected with pressure except the internal strain parameter and Poisson's ratio. The mechanical stability criteria for the materials of interest for pressure up to 120 Kbar are fulfilled. The considered materials can be used in optoelectronic devices. The overall agreement between our results and the available experimental and theoretical data is found to be reasonable good. Our calculated values may serve as a reference, especially for high pressure.

Keywords Pressure · Mechanical properties · AlP and AlSb semiconductors

1 Introduction

Special attention has been given to the electronic and optical properties of semiconductors because they are one of the best tools for guiding the successful design and fabrication of optoelectronic devices. Recently, III-V zinc blende semiconductors have become an important area for many device applications of high-speed electronic and long-wavelength like diode lasers, light-emitting diodes, high-electron-mobility and hetero-structure, photo-detectors and electro-optic modulators [1–4]. The physical properties of III–V compounds have been studied extensively in recent years and a large amount of information is now available both experimentally and theoretically [4].

AlSb is an indirect-gap semiconductor with a lattice constant only slightly larger than that of GaSb. In recent years it has found considerable use as the barrier material in high mobility electronic and long-wavelength optoelectronic devices [4]. The effect of strain on electronic properties of the studied compounds requires knowledge of their mechanical properties, specifically the elastic constants which describe the response to an applied macroscopic stress. So, the mechanical properties of a semiconductor are of particular interest for its applications [5].

Jappor et al have been investigated the effect of pressure on the structural and electronic parameters of zinc-blende aluminum phosphide crystal [6]. The effect of temperature and pressure on the electronic, optical and mechanical properties of different semiconductor materials has been calculated by Degheidy and Elkenany [7–11]. Joshi et al have been calculated the charge density and electronic band structures for $Ga_xAl_{1-x}Sb$ with x = 1:0, 0.5 and 0.0 [12]. The high-pressure phase diagrams of AlP, AlAs, and AlSb have been studied by Mujica et al [13]. The structural and dielectric properties of AlN under pressure have been calculated by Saib et al [14]. Harrison has been studied the quantum wells wires and quantum dots [15]. Elabsy and Elkenany have been calculated thermal response to electronic structures of bulk semiconductors [16]. The pressure dependence of energy gap of III–V and II–VI ternary semiconductors has been determined by Dongguo and Ravindra [17]. Wang et al have been investigated the pressure dependence of elastic and dynamical properties of zinc-blende ZnS and ZnSe from first principle calculation [18]. Dinesh et al have been determined the pressure dependence of elastic properties of ZnX (X = Se, S and

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Te) [19]. The properties of Group IV, III–V and II–VI semiconductors have been studied by Adachi [20].

The main motivation for the present work is to study the change in the mechanical properties of AlP and AlSb under hydrostatic pressure. The studied mechanical parameters are the elastic constants (c_{ij}) and their related elastic moduli, as bulk (B_u), shear (S_h) and Young (Y_0) of these compounds. Another interesting parameters like, Poisson's ratio (σ) linear compressibility (C_0), Cauchy ratio (C_a), anisotropy factor (A), bond stretching (α), bond binding force (β), internal strain parameter (ζ) and transverse effective charge (e_T^*) have been investigated under pressure. Our calculations are performed using the (EPM) and the results are found in good agreement with the available experimental and theoretical data.

2 Computational Method

The calculations presented in this work were performed using (EPM). The energy eigenvalues of AlP and AlSb are calculated by solving the one-electron Schrodinger equation

$$\left[\frac{-\hbar^2}{2m}\nabla^2+\mathrm{V(r)}\right]\psi_{\mathrm{n},\mathbf{k}}(\mathbf{r}) = \mathrm{E}_{\mathrm{n},\mathbf{k}}\,\psi_{\mathrm{n},\mathbf{k}}(\mathbf{r}) \tag{1}$$

where $\mathrm{V}(\mathbf{r})$ is the crystalline pseudo-potential, $\psi_{\mathrm{n},\mathbf{k}}(\mathbf{r})$ are the pseudo-wave functions and $E_{n,\mathbf{k}}$ are the corresponding energy eigen-values. For the case of zinc-blende structure, it is convenient to express $\mathrm{V}(\mathbf{G})$ in terms of atomic pseudo potential form factors as [15]

$$V(\mathbf{G}) = w^s(\mathbf{G})\cos(\mathbf{G}.\tau) + i\,w^a(\mathbf{G})\sin(\mathbf{G}.\tau), \tag{2}$$

where W^s and W^a are the symmetric and anti-symmetric form factors that are fitted empirically to achieve the close agreement to the experimental energy band gaps, τ is the position vector of each atom in the unit cell and equal to $\frac{a}{8}(1,1,1)$, where a is the lattice constant of the studied material. The basis states used to form the hamiltonian matrix consist of plane waves with wave vectors $\mathbf{G}+\mathbf{k}$, where $\mathbf{k}$ is a wave vector lying within the first Brillouin zone and $\mathbf{G}$ are the reciprocal lattice vectors, The Schrodinger equations solved by determining the roots of the secular equation derived from the hamiltonian matrix,

$$\left\|\frac{1}{2}\left|\vec{k}+\vec{G}'\right|^2 - E_{nk}(p) + \sum_{\vec{G}\neq\vec{G}'} V\left(\left|\Delta\vec{G},p\right)\right\| = 0\,, \tag{3}$$

$$where\ V(\Delta\vec{G},p) = W^s(\Delta\vec{G},p)\cos(\Delta\vec{G}\bullet\vec{\tau}) + iW^a(\Delta\vec{G},p)\sin(\Delta\vec{G}\bullet\tau) \tag{4}$$

is the pressure-dependent pseudo-potential with $\Delta\vec{G}=\vec{G}-\vec{G}'$. The pseudo-potential form factors have been deduced by fitting the band-gap energies of AlP and AlSb at some specific high symmetric points,$\Gamma(0,0,0)$, L(0.5,0.5,0.5), X(0,0,1), in the Brillouin zone to the experimental data available from the literature. The dimension of our eigenvalue problem is a (65× 65) matrix which gives generally good convergence. The energy band gaps E_g^Γ, E_g^L and E_g^X are determined by arranging the calculated energy eigenvalues $E_{nk}(p)$ and setting the top of the valance band as a reference. The energy band gaps are the difference between the top of valence band and the minimum of conduction band (E_g^Γ at Γpoint, E_g^L at L point and E_g^X at X point). The experimental data regarding the energy band gaps and lattice constants for AlP and AlSb at various values of pressure used in the fitting procedure are obtained from empirical relations found in reference [20]. The final adjusted symmetric $W^s(\Delta\vec{G},p)$ and anti-symmetric $W^a(\Delta\vec{G},p)$ form factors at G(1,1,1) are used to calculate the polarities (α_p) of the studied compounds by using Vogl's relation [21]. Knowledge of the polarities, the elastic constants $C_{ij}(p)$, and their related moduli, like bulk $B_u(p)$, shear $S_h(p)$ and Young $Y_0(p)$ of AlP and AlSb could be determined [22, 23]. Other important quantities as Poisson ratio $\sigma(p)$, linear compressibility $C_0(p)$, Cauchy $C_a(p)$ ratio, bond stretching $\alpha(p)$, bond-bending force $\beta(p)$ and internal-strain parameter $\zeta(p)$ for the studied materials could be also successfully calculated.

3 Results and Discussion

The energy band gaps E_g^Γ, E_g^L and E_g^X of AlP and AlSb at various values of pressure are determined by solving the secular determinant (3) and listed in Table 1 and displayed in Fig. 1. Our results show that both compounds are indirect semiconductors (X) over the whole region of pressure (0-120 Kbar). The energy band gaps E_g^Γ and E_g^L of AlP are slightly increased with increasing pressure, while E_g^X is linearly decreased. Our calculated energy band gaps are found in excellent agreement with the available experimental data [4, 20]. Table 1 contains also the lattice constants of AlP and AlSb using in our calculations. The behavior of these energy gaps for AlP and AlSb under pressure can be fitted by the following polynomials:

For AlP

$$E_g^L(p) = 3.5225 + 0.0002p - 7\times10^{-7}p^2 \tag{5}$$

$$E_g^\Gamma(p) = 3.5419 + 0.0003p + 4\times10^{-7}p^2 \tag{6}$$

$$E_g^x(p) = 2.48 - 0.0016p \tag{7}$$

For AlSb

$$E_g^L(p) = 2.1923 + 0.0053p - 5\times10^{-5}p^2 \tag{8}$$

Table 1 Lattice constants and energy band gaps of AlP and AlSb at various values of pressure

p	AlP				AlSb			
	a(p) (a.u.)	E_g^L (eV)	E_g (eV)	E_g^X (eV)	a(p) (a.u.)	E_g^L (eV)	E_g eV)	E_g^X(eV)
0	10.3241	3.5225, 3.57[a]	3.5419, 3.6[a]	2.48, 2.45[a]	11.5939	2.1923, 2.21[a]	2.2162, 2.215[b]	1.61, 1.61[b]
20	10.2450	3.5272	3.5491	2.4480, 2.4480[b]	11.4712	2.2794	2.4077, 2.4054[b]	1.5256, 1.5256[b]
40	10.1741	3.5300	3.5543	2.4160, 2.4160[b]	11.3651	2.3267	2.5524, 2.5526[b]	1.4404, 1.4404[b]
60	10.1101	3.5302	3.5576	2.3840, 2.384[b]	11.2718	2.3412	2.6577, 2.6566[b]	1.3544, 1.3544[b]
80	10.0516	3.5320	3.5631	2.3520, 2.352[b]	11.1886	2.3131	2.7165, 2.7174[b]	1.2676, 1.2676[b]
100	9.9979	3.5349	3.5722	2.3200, 2.3200[b]	11.1135	2.2570	2.7314, 2.7350[b]	1.18, 1.18[b]
120	9.9482	3.5355	3.5786	2.2880, 2.2880[b]	11.0453	2.1444	2.7070, 2.7094[b]	1.0916, 1.0916[b]

[a]Ref. [4], [b]Ref. [20]

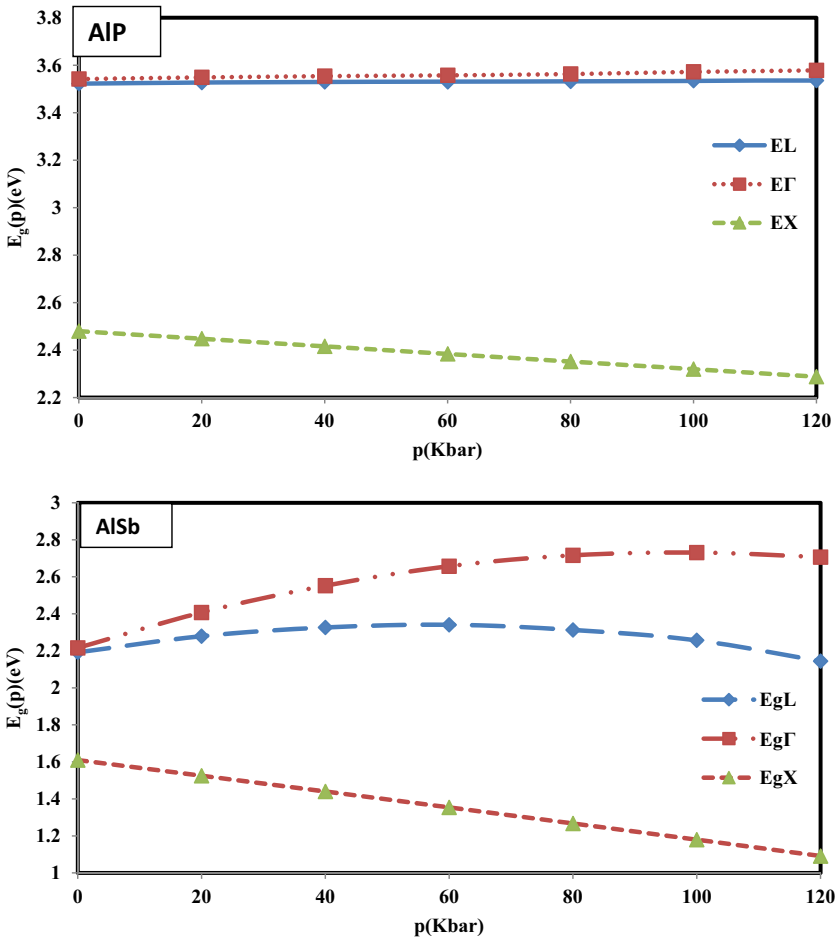

Fig. 1 The energy band gaps of AlP and AlSb as function of pressure

Table 2 Polarity (α_p), Elastic constants (C_{11}, C_{12} and C_{44}), Bulk modulus (B_u), Young's modulus (Y_0) and Shear modulus (S_h) of AlP and AlSb at different values of pressure

p(Kbar)	AlP							AlSb						
	α_p	(10^{11}dyn/cm^2)						α_p	(10^{11}dyn/cm^2)					
		c_{11}	c_{12}	c_{44}	B_u	Y_0	S_h		c_{11}	c_{12}	c_{44}	B_u	Y_0	S_h
0	0.4094, 0.40[a]	13.202, 13.37[a]	5.7564, 5.83[a]	5.3121, 5.763[b]	8.2384, 8.252[b]	9.7068, 11.254[b]	3.7230, 4.421[b]	0.2405, 0.24[c]	8.9324, 8.93[c]	3.8500, 3.85[c]	3.6111, 4.07[d]	5.5441, 5.8[d]	6.6132, 5.9[d]	2.5412, 2.2[d]
20	0.4104	13.700	5.9738	5.5121	8.5492	10.072	3.8630	0.2436	9.3980	4.0512	3.7992	5.8335	6.9574	2.6734
40	0.4105	14.180	6.1833	5.7053	8.8489	10.425	3.9984	0.2478	9.8116	4.2303	3.9661	6.0908	7.2627	2.7907
60	0.4114	14.615	6.3736	5.8801	9.1208	10.744	4.1208	0.2502	10.205	4.4004	4.1248	6.3352	7.5533	2.9022
80	0.4114	15.046	6.5615	6.0535	9.3897	11.061	4.2423	0.2534	10.562	4.5550	4.2689	6.5573	7.8169	3.0034
100	0.4117	15.447	6.7366	6.2148	9.6402	11.356	4.3553	0.2559	10.901	4.7016	4.4055	6.7679	8.0669	3.0995
120	0.4121	15.827	6.9027	6.3676	9.8776	11.635	4.4623	0.2559	11.241	4.8486	4.5433	6.9795	8.3191	3.1964

[a]Ref. [24], [b]Ref. [25], [c]Ref. [26], [d]Ref. [27]

$$E_g^{\Gamma}(p) = 2.2162 + 0.0106p - 5 \times 10^{-5} p^2 \quad (9)$$

$$E_g^{x}(p) = 1.61 - 0.0042p - 1 \times 10^{-6} p^2 \quad (10)$$

The polarity (α_p) and the elastic constants (C_{11}, C_{12} and C_{44}) of AlP and AlSb at different values of pressure are listed in Table 2 and displayed in Fig. 2. The results show that the elastic constants of both compounds have the same behaviors, they are slightly increased with increasing pressure; however, the increasing rate of C_{11} is higher than those of C_{12} and C_{44}. Knowledge of the elastic constants,

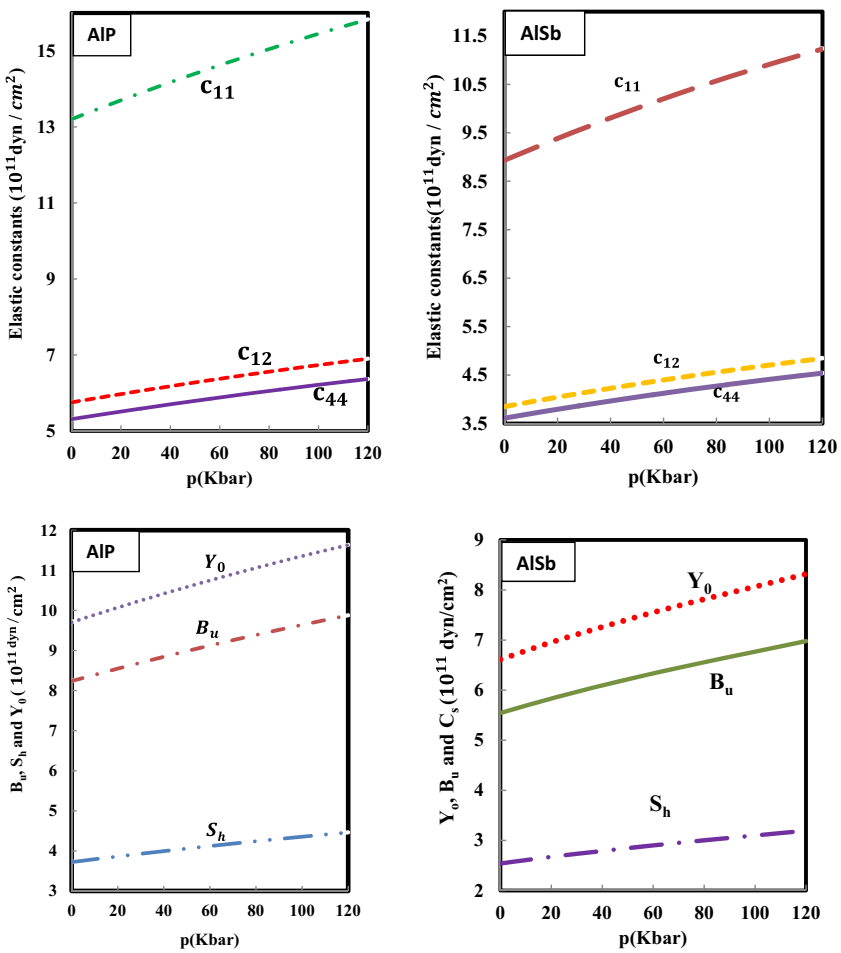

Fig. 2 Elastic constants($C_{11}C_{12}andC_{44}$), Bulk modulus (B_u), Young's modulus(Y_0) and Shear modulus (S_h) of AlP and AlSb as function of pressure

Table 3 Poisson's ratio (σ), linear compressibility (C_0), Cauchy ratio (C_a) and anisotropy factor (A) for AlP and AlSb at various values of pressure

p(Kbar)	AlP				AlSb			
	σ	$C_0(10^{-13}cm^2/dyn)$	C_a	A	σ	$C_0(10^{-13}cm^2/dyn)$	C_a	
0	0. 3036, 0.272[a]	4. 0461, 3.59[b]	1.0836, 1.05[b]	0.7008, 0.702[b]	0. 3012, 0.331[b]	6. 0124, 5.73[b]	1.0661, 1.07[b]	0.7037, 0.543[b]
20	0. 3036	3.8990	1.0838	0.7008	0. 3012	5.7141	1.0663	0.7037
40	0. 3036	3.7669	1.0838	0.7008	0. 3013	5.4728	1.0666	0.7036
60	0. 3037	3.6546	1.0839	0.7008	0. 3013	5.2616	1.0668	0.7036
80	0. 3037	3.5500	1.0839	0.7008	0. 3013	5.0834	1.0670	0.7036
100	0. 3037	3.4578	1.0840	0.7008	0. 3013	4.9252	1.0672	0.7035
120	0. 3037	3. 3747	1.0840	0.7008	0. 3013	4. 7759	1.0672	0.7035

[a]Ref. [25], [b]Ref. [20]

the bulk (B_u), shear (S_h) and Young's (Y_0) moduli of AlP and AlSb are calculated and listed in Table 2. All calculated values in Table 2 at normal pressure are compared with the experimental and theoretical data and showed good agreement [24–27]. The variation of B_u, S_h and Y_0 of AlP and AlSb with pressure is displayed in Fig. 2. As pressure increases, the elastic moduli B_u, S_h and Y_0 of AlP and AlSb increase monotonically with approximately the same rate, however, the elastic moduli of AlP have higher values than those of AlSb.

The fitting polynomial relations for the elastic constants (C_{11}, C_{12}, C_{44}) and elastic moduli (B_u, S_h, Y_0) for AlP and AlSb with pressure are given by the following relations:

For AlP

$$C_{11}(p) = 13.202 + 0.0255p - 3 \times 10^{-5} p^2 \quad (11)$$

$$C_{12}(p) = 5.7564 + 0.0111p - 1 \times 10^{-5} p^2 \quad (12)$$

$$C_{44}(p) = 5.3121 + 0.0102p - 1 \times 10^{-5} p^2 \quad (13)$$

$$S_h(p) = 3.723 + 0.0072p - 8 \times 10^{-6} p^2 \quad (14)$$

$$B_u(p) = 8.2384 + 0.0159p - 2 \times 10^{-5} p^2 \quad (15)$$

$$Y_0(p) = 9.7068 + 0.0187p - 2 \times 10^{-5} p^2 \quad (16)$$

For AlSb

$$C_{11}(p) = 8.9324 + 0.0232p - 3 \times 10^{-5} p^2 \quad (17)$$

$$C_{12}(p) = 3.85 + 0.01p - 1 \times 10^{-5} p^2 \quad (18)$$

$$C_{44}(p) = 3.6111 + 0.0094p - 1 \times 10^{-5} p^2 \quad (19)$$

$$S_h(p) = 2.5412 + 0.0066p - 1 \times 10^{-5} p^2 \quad (20)$$

$$B_u(p) = 5.5441 + 0.0144p - 2 \times 10^{-5} p^2 \quad (21)$$

$$Y_0(p) = 6.6132 + 0.0171p - 2 \times 10^{-5} p^2 \quad (22)$$

The Poisson ratio σ), linear compressibility (C_0), Cauchy ratio C_a and anisotropy factor (A) for AlP and AlSb at various values of pressure are calculated and listed in Table 3. It is seen from this table that σ ,C_a and A are not

Table 4 Bond- stretching α), bond- bending (β) force internal strain parameter (ζ) for AlP and AlSb at different values of pressure

p(Kbar)	AlP				AlSb			
	α(N/m)	β(N/m)	ζ	e_T^*	α(N/m)	β(N/m)	ζ	e_T^*
0	41.620, 43.25a	10.170, 10.19[a]	0.6073, 0.618[b]	2.4025, 2.38[a]	31.417, 31.89[c]	7.7958, 7.74[c]	0.6024, 0.635[b]	1.9094, 1.91[c]
20	42.860	10.472	0.6073	2.4050	32.707	8.1144	0.6024	1.9198
40	44.056	10.764	0.6073	2.4052	33.835	8.3920	0.6025	1.9339
60	45.124	11.024	0.6073	2.4074	34.904	8.6559	0.6026	1.9418
80	46.186	11.283	0.6073	2.4074	35.862	8.8917	0.6026	1.9524
100	47.165	11.522	0.6073	2.4081	36.766	9.1144	0.6027	1.9607
120	48.086	11.746	0.6074	2.4091	37.683	9.3417	0.6027	1.9607

[a]Ref. [24],[b]Ref. [28], [c]Ref. [29]

affected with pressure, however, C_0 is slightly decreased with increasing pressure. All calculated values in Table 3 at p=0 Kbar showed good agreement with the available experimental data [20, 25, 26].

Table 4 shows the effect of pressure on the calculated values of bond- stretching (α), bond- bending (β) force constant and internal strain parameter (ζ) of AlP and AlSb. From this table, we show that α and β for both compounds are increased slightly with pressure, however ζ is not affected. The calculated quantities at p=0 Kbar are found in good agreement with the available experimental data [24, 28, 29]. The elastic constants may help in getting information about the mechanical stability of the considered compounds under pressure. A given crystal structure cannot exist in a stable or meta stable phase unless its elastic constants obey certain relationships. The mechanical stability criteria of the crystal are $C_{11}(p) + 2C_{12}(p) > 0$, $C_{44}(p) > 0$, $C_{11}(p) - |C_{12}(p)| > 0$ [30–32], we observed from our calculated results that these conditions are fulfilled over the whole region of pressure (0-120 Kbar) reflecting that AlP and AlSb have more stability in its zinc-blende structure under the studied region.

4 Conclusions

In this study, we used the (EPM) in our calculations, the direct and indirect energy gaps of AlP and AlSb are first calculated at different values of pressure. The polarity of the studied compounds are calculated from the adjusted symmetric and anti-symmetric form factors at G(1,1,1). The elastic constants C_{11}, C_{12} and C_{44} and their related elastic parameters, namely bulk (B_u), shear (S_h) and Young's (Y_0) moduli and their variation under pressure have been investigated. Another important parameters as bond-stretching (α), bond-bending force constants (β), internal-strain parameter (ζ), Poisson's ratio (σ), linear compressibility (C_0), Cauchy ratio (C_a) and anisotropy factor (A) are determined at different values of pressure. Our results at p = 0 Kbar are showed good agreement within the range values known from the available experimental and published data.

References

1. Iga K, Kinoshita S (1996) Process technology for semiconductor lasers. Springer, Berlin
2. Quillec M (1996) Materials for optoelectronics. Kluwer Academic, Boston
3. Levinshtein M, Rumyantsev S, Shur M (1999) Handbook series on semiconductor parameters, vol 2. World Scientific, Singapore
4. Vurgaftman I, Meyer JR, Ram-Mohan LR (2001) J Appl Phys 89:5815
5. Hannachi L, Bouarissa N (2009) Phys B 404:3650
6. Hamad Jappor R, Mudar Abdulsattar A, Ahmed Abdul-Lettif M (2010) Open Cond Matter Phys J 3:1–7
7. Degheidy AR, Elkenany EB (2013) Mater Chem Phys 143:1
8. Degheidy AR, Elkenany EB (2012) Math Sci Semicond Process 15:505
9. Degheidy AR, Elkenany EB (2012) Chin Phys B 21:12
10. Degheidy AR, Elkenany EB (2011) Semiconductors 45:10
11. Degheidy AR, Elabsy AM, Elkenany EB (2012) Superlattice Microstruct 52:336
12. Joshi KB, Nishant Patel N (2008) PRAMANA. J Phys 70:295–305
13. Mujica A, Rodri Âguez-Hernândez P, Radescu S, Needs RJ, Munõz A (1999) Phys Stat Sol (B) 39:211
14. Saib S, Bouarissa N, Rodríguez-hernández P, Munõz A (2008) Physica B 403:4059–4062
15. Harrison P (2005) Quantum wells wires and quantum dots, 2nd edn. Wiley, New York
16. Elabsy AM, Elkenany EB (2010) Phys B 405:266
17. Dongguo C, Ravindra NM (2012) J Mater Sci 47:5735–5742
18. Wang HY, Cao J, Huang XY, Huang JM (2012) Cond Matter Phys 15(1, 13705):1–10
19. Varshney D, Sharma P, Kaurav N, Singh RK (2005) Bull Mater Sci 28:651–661
20. Adachi S (2005) Properties of group IV, III–V and II–VI semiconductors. Wiley, Hoboken
21. Vogl P (1978) J Phys 11:251
22. Bouarissa N (2006) Mater Chem Phys 100:41
23. Baranowski JM (1984) J Phys 17:6287
24. Zerroug S, Ali Sahraoui F, Bouarissa N (2006) Mater Lett 60:546–550
25. Bouhemadou A, Ghebouli MA, Ghebouli B, Fatmi M, Bin-Omran S, Ucgun E, Ocak HY (2013) Mater Sci Semicond Process 16:718–726
26. Gueddim A, Zerdoum R, Bouarissa N (2006) Mater Sci Eng B 131:111–115
27. Martin RM (1970) Phys Rev B 1:4005
28. de Gironcoli S, Baroni S, Resta R (1989) Phys Rev Lett 62:2853
29. Kim K, Lambrecht WRL, Segall B (1996) Phys Rev B 53:16310
30. Daoud S, Bioud N, Bouarissa N (2015) Mater Sci Semicond Process 31:124–130
31. Aouina NY, Mezrag F, Boucenna M, El-Farra M, Bouarissa N (2005) Mater Sci Eng B 123:87–93
32. Saib S, Bouarissa N (2006) Solid State Electron 50:763–768