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Electronic, optical, and mechanical properties of $Al_xIn_{1-x}P$ alloys under temperature and pressure

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Abstract
In this work, the optoelectronic and mechanical properties of $Al_xIn_{1-x}P$ combinations in the zinc-blende structure were studied for different Al concentrations. The energy band gaps $\left(E_g^L, E_g^\Gamma, E_g^X\right)$, refractive index (n), high frequency and static dielectric constants (ε_∞, ε_o), elastic parameters (C_{11}, C_{12}, C_{44}) were investigated. Other mechanical properties such as bulk (B_u), shear (C_s), Young's (Y_0) moduli, Poisson ratio (σ), linear compressibility (C_o), Cauchy (C_a) ratio, isotropy factor (A), bond stretching parameter (α), bond-bending force parameter (β), internal-strain parameter (ξ), and the transverse effective charge (e_T^*) were calculated. Also, the temperature and pressure dependences of these properties were studied. Our estimations were made with the empirical pseudo-potential method combined with the virtual crystal approximation incorporated the compositional disorder impact. There was a reasonable agreement between our determined outcomes and the accessible experimental values for the binary materials AlP and InP which give help for the consequences of the ternary combinations.

Keywords Mechanical properties · Electronic properties · Optical properties · Temperature · Pressure

1 Introduction

The alloys of III–V zinc-blende semiconductor compounds are of vital importance because these materials are potentially good for the application of optoelectronic and high-speed electronics (Ohnuma et al. 2000). The Al_xIn_{1-x} P is a wide bandgap III–V semiconductor alloy which is motivating due to its least index of refraction between other As or P

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semiconductor composites (Ishitani et al. 1997; Munns et al. 1993). It very well may be used for photovoltaic devices, light-emitting diodes in the visible spectral range, and high-performance laser diodes (Bour et al. 1987; Christian et al. 2013; Dai et al. 2015; Lin et al. 2015; Tukiainen et al. 2006; Zhang et al. 2010). Also, $Al_xIn_{1-x}P$ is regularly utilized as a window layer of semiconductor solar cell combinations (Abdollahi et al. 2016; Corkish and Green 1993). The alloying technique prompts critical variations in the lattice parameters, distribution of electronic charge.

The study of semiconductor behavior under high temperatures has become a critical subject showing important development (Degheidy and Elkenany 2015). Various authors have reported the temperature dependence of the energy gaps for certain semiconductors, both theoretically (Degheidy et al. 2012; Fan 1951; Keffer et al. 1970; Tsang and Cohen 1971) and experimentally (Pandey and Phillips 1974; Skelton et al. 1972; Walter and Cohen 1970, 1969). The examined alloy $Al_xIn_{1-x}P$ has consisted of two binary materials AlP and InP. Probably the simplest approaches to change the electronic and structural properties of the ternary combination are changeable of the compositional content, going from 0 to 1. A few techniques have been created to figure the band structure of semiconductors, between them is the EPM (Chelikowsky and Cohen 1976; Degheidy et al. 2012, 2021a, b; Elkenany 2021a, b, c; Elkenany and Othman 2021; Al Maaitah and Elkenany 2022; Pandey and Phillips 1974; Phillips and Pandey 1973). There is also a wonderful method for calculating the electronic, optical, and mechanical properties of semiconductor materials which is the density functional theory (DFT) (Al-Douri et al. 2015; Bouhemadou et al. 2019; Moakafi et al. 2008; Ouahrani et al. 2010; Reshak et al. 2011). The examination of pressure and temperature reliance of electronic, optical, and mechanical properties in semiconductors has been the object of numerous investigations (Chen and Ravindra 2012; Degheidy et al. 2018a, 2017, 2012; Degheidy and Elkenany 2012, 2013a, b, c, 2017; Elkenany 2016; Jappor et al. 2010; Saib et al. 2008; Wang et al. 2012).

In the current study, the electronic properties such as the energy bandgaps $\left(E_g^L, E_g^\Gamma E_g^X\right)$, optical properties such as refractive index, dielectric constants (n, ε_∞, ε_o) and mechanical properties such as elastic constants (C_{11}, C_{12}, C_{44}), bulk, shear and Young's moduli (B_u, C_s, Y_0) for $Al_xIn_{1-x}P$ alloys have been calculated. The Poisson ratio (σ), linear compressibility (C_o), Cauchy ratio (C_a), anisotropy factor (A), bond stretching parameter (α), bond-bending force parameter (β), internal-strain parameter (ξ), and the transverse effective charge (e_T^*) for $Al_xIn_{1-x}P$ alloys were determined. The temperature, pressure, and composition dependence of the considered alloy for the studied properties has been studied. Our calculations were matched with the available published data especially for binary AlP and InP compounds and showed very good agreement which gives support for the results of the $Al_xIn_{1-x}P$ ternary alloys.

2 Theory and calculations

The electronic structure of the alloys $Al_xIn_{1-x}P$ was determined using the EPM. The alloy potential was calculated using the $V_{VCA}(\mathbf{r})$ beside $V_{dis}(\mathbf{r})$ due to the compositional disorder (Bouarissa and Aourag 1995; Lee et al. 1990)

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

where the potentials in Eq. (1) have the formats (Bouarissa and Aourag 1995; Lee et al. 1990)

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

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

where x is the Aluminum concentration (Al) and Ω is treated as an adjustable parameter. The x-dependent form factors of the considered ternary alloys at a constant T and p could be given in the form

$$W^{S,A} = xW^{S,A}_{AlP} + (1-x)W^{S,A}_{InP} - \sqrt{x(1-x)}\left[W^{S,A}_{AlP} - W^{S,A}_{InP}\right] \tag{4}$$

where $W^{S,A}_{AlP}$, $W^{S,A}_{InP}$ are the symmetric and anti-symmetric form factors of the AlP and InP, respectively. The lattice constant of $Al_xIn_{1-x}P$ alloy was acquired by the Vegard's relation (Vegard 1921)

$$a_{alloy} = (1-x)a_{InP} + xa_{AlP} \tag{5}$$

where $a_{AlP} and a_{InP}$ are the lattice constants of the associated compounds AlP and InP, respectively. Knowing the lattice constants and the form factors of $Al_xIn_{1-x}P$ alloy at a constant composition parameter, the energy eigenvalues $E_{n\mathbf{k}}(x)$ were calculated by solving numerically the secular determinant (Fan 1951; Keffer et al. 1970)

$$\left\| \frac{1}{2}\left|\vec{k} + \vec{G}'\right|^2 - E_{nk} + \sum_{\vec{G}\neq\vec{G}'} V(\left|\Delta\vec{G}\right) \right\| = 0 \tag{6}$$

where

$$V(\left|\Delta\vec{G}\right) = W^s(\Delta\vec{G})\cos(\Delta\vec{G}\bullet\vec{\tau}) + iW^a(\Delta\vec{G},x)\sin(\Delta\vec{G}\bullet\tau)$$

is the pseudo-potential and τ is the atomic position and equals to $\frac{a}{8}(1,1,1)$. The calculated values of the fundamental energy band gaps of $Al_xIn_{1-x}P$ alloy were utilized to determine n (Moss 1950) and the ε_∞ by applying the Samara relation (Samara 1983)**.** The gained W^S and W^A at G(1,1,1) were utilized to determine the α_p using Vogl's relation (Vogl 1978) as

$$\alpha_p = -\frac{w_3^A}{w_3^S} \tag{8}$$

The elastic constants at constant T and p were given by Refs. (Bouarissa 2003; Munns et al. 1993; Shen 1994). The knowledge of the C_{11}, C_{12}, and C_{44} permitted us to calculate B_u, C_s and Y_o of $Al_xIn_{1-x}P$ alloys (Cahn and Cohen 1970; Pandey and Phillips 1974; Walter and Cohen 1969). Other significant parameters as the ratio σ, C_o, C_a and A were also successfully calculated (Bouarissa 2003; Shen 1994). Finally, the α, β, ξ and e_T^* for the studied alloys have been determined (Bouarissa 2003; Walter and Cohen 1969).

3 Results and discussions

3.1 Effect of Al concentration

The variation of the calculated E_g^L, E_g^Γ, E_g^X with Al content in $Al_xIn_{1-x}P$ is recorded in Table 1 and shown in Fig. 1. It was seen that E_g^Γ and E_g^L are raised with different rates with increasing Al content, however, E_g^X is increased with a weaker rate. We noted that $Al_xIn_{1-x}P$ is a direct semiconductor and changed to an indirect one at about x = 0.36. This result is in good accord with that mentioned by Vurgaftman et al. (Vurgaftman et al. 2001) who proposed that this material has a direct energy bandgap for x < 0.44. The utilization of the improved VCA in our computations of $Al_xIn_{1-x}P$ introduced the optical bowing parameters as −1.6 eV, −0.49 eV, and 0.27 eV at L, Γ, and X, respectively. Our calculated values of the optical bowing parameters are in excellent agreement with the published values of −1.7 eV, −0.48 eV, and 0.3 eV, respectively as in Refs. (Mezrag and Bouarissa 2018; Vurgaftman et al. 2001), justifying the reliability of our calculated method and results. The studied E_g^L, E_g^Γ, E_g^X were compared with the published ones and indicated fantastic agreement (Adachi 2005, 1987; Tiwari and Frank 1992; Vurgaftman et al. 2001). The variation of these energy gaps with concentration could be shaped by the following polynomials:

$$E_g^L = 2.0552 + 3.2277\,x - 1.6015\,x^2 \tag{9}$$

$$E_g^\Gamma = 1.358 + 2.7848\,x - 0.4931\,x^2 \tag{10}$$

Table 1 The E_g^L, E_g^Γ and E_g^X of $Al_xIn_{1-x}P$ at T = 300 K and $p = 0$ Kbar for different x

x	E_g^L(eV)	E_g^Γ(eV)	E_g^X(eV)
0	2.0552, 2.05[b]	1.3580, 1.35[b], 1.3582[a]	2.2421, 2.21[b]
0.1	2.2462	1.5451	2.2169
0.2	2.5402	1.8280	2.2342
0.3	2.8193	2.1077	2.2643
0.4	3.0703	2.3781	2.3017
0.5	3.2871	2.6373	2.3425
0.6	3.4648	2.8837	2.3841
0.7	3.5976	3.1141	2.4244
0.8	3.6767	3.3213	2.4620
0.9	3.6871	3.4891	2.4964
1	3.5785, 3.5378[c], 3.57[c]	3.5692, 3.5527[c], 3.6[d], 3.56[e]	2.5460, 2.4878[c], 2.5[c], 2.45[d], 2.52[e]

[a]Ref. (Adachi 2005)

[b]Ref.(Adachi 1987)

[c]Ref.(Vurgaftman et al. 2001)

[d]Ref.(Tiwari and Frank 1992)

[e]Ref.(Mezrag and Bouarissa 2018)

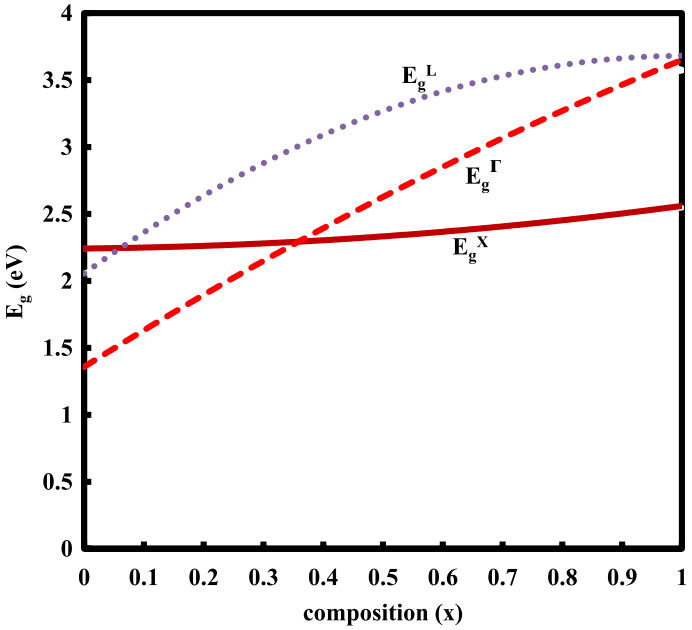

Fig. 1 Energy band gaps of $Al_xIn_{1-x}P$ at T = 300 K& $p = 0$ Kbar as function of concentration

$$E_g^X = 2.2421 + 0.0438\,x + 0.2742\,x^2 \tag{11}$$

Figure 2 displays the variation of refractive index (n), optical and static dielectric constants (ε_∞, ε_o) of $Al_xIn_{1-x}P$ with composition at T = 300 K and $p = 0$ Kbar. It was seen that

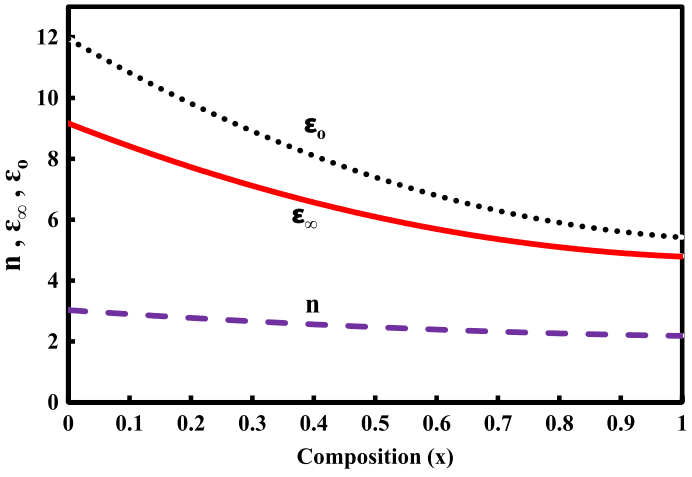

Fig. 2 The refractive index (n), optical and static dielectric constants (ε_∞, ε_o) of $Al_xIn_{1-x}P$ as function of Al content at T = 300 K & $p = 0$ Kbar

the refractive index is slightly linear decreased with enhancing composition. It was also found that the optical and static dielectric constants (ε_∞, ε_o) are decreased nonlinearly with increasing the Al content. This is due to the inverse relationship between the energy band gap and the refractive index.

The polarities α_p, C_{11}, C_{12}, C_{44}, B_u, $C_{s,}$ and Y_0 of $Al_xIn_{1-x}P$ at various concentrations are recorded in Table 2 and offered in Fig. 3. A good agreement was obtained between our results and the published data as in Refs. (Bour et al. 1987; Christian et al. 2013; Keffer et al. 1970; Munns et al. 1993; Ohnuma et al. 2000). We noted that the elastic parameters (C_{11}, C_{12}, and C_{44}) are enhanced nonlinearly with increasing the Al concentration. From Fig. 3, we observed that the change rate with the composition of C_{12}, C_{44} is small compared to that with C_{11}. It was observed that the change of the elastic moduli B_u, $C_{s,}$ and Y_0 with composition has similar behavior to the elastic constants. This means that the bulk, shear, and Young's moduli are increased with enhancing the Al content.

The study of mechanical properties enables us to classify and identify the materials. Also, it defines a material's extent of usefulness and determines the service life that can be predicted. The Poisson ratio (σ), linear compressibility (C_o), Cauchy (C_a) ratio, Born ratio (B_0), anisotropy factor (A), bond stretching parameter (α), bond-bending force parameter (β), internal-strain parameter (ξ), the transverse effective charge (e_T*), and effective charge (Z*) of $Al_xIn_{1-x}P$ at different values of Al content are listed in Table 3. The comparison between our calculations and the available published data is found to be very good agreement (Bour et al. 1987; Christian et al. 2013; Ishitani et al. 1997; Keffer et al. 1970; Ohnuma et al. 2000; Tan et al. 2010; Tsang and Cohen 1971). It was observed that the α and β are enhanced with enhancing Al concentration, C_0 is reduced with raising Al content, while the other parameters in the table are very marginally influenced with Al concentration in $Al_xIn_{1-x}P$ alloy.

3.2 Influence of pressure and temperature

In this section, the influence of temperature (0–600 K) and pressure (0–120 Kbar) on the considered properties of $Al_xIn_{1-x}P$ with a constant concentration (x = 0.5) were determined. The E_g^L, E_g^Γ and E_g^X of $Al_{0.5}In_{0.5}P$ versus temperature and pressure are recorded in Table 4 and exhibited in Fig. 4. We found that all the band gaps of $Al_{0.5}In_{0.5}P$ are decreased with enhancing temperature. We also found that the E_g^X is linearly decreased, while E_g^Γ and E_g^L are increased with increasing pressure. It was observed that the $Al_{0.5}In_{0.5}P$ is an indirect semiconductor alloy within the entire range of temperature and pressure.

The determined polarities α_p, C_{11}, C_{12}, C_{44}, B_u, $C_{s,}$ and Y_0 of $Al_{0.5}In_{0.5}P$ at different estimations of temperature and pressure are listed in Table 5 and presented in Fig. 5. It was found that the C_{11}, C_{12}, C_{44}, B_u, $C_{s,}$ and Y_0 are slightly influenced by temperature. Also, it was found that these parameters are increased with enhancing pressure. Due to the lack of published data, our calculated data of C_{11}, C_{12}, C_{44}, B_u, $C_{s,}$ and Y_0 of $Al_{0.5}In_{0.5}P$ alloy at high temperatures and pressures may serve as a prediction for future experimental works. The analysis of the elastic constants could help to obtain data about the stability of the crystal. The mechanical stability requirements of a cubical crystal were given by Ref. (Bouarissa 2003) as $(C_{11}+2C_{12})>0$, $C_{44}>0$, $(C_{11}-C_{12})>0$. Our study confirms that the conditions are satisfied at the numerous values of temperatures (0–600 K) and pressures from (0–120 Kbar) which indicates the stability of $Al_xIn_{1-x}P$ in its structure.

The calculated Poisson ratio (σ), linear compressibility (C_0), Cauchy ratio (C_a), Born ratio (B_0), anisotropy factor (A), bond stretching parameter (α), bond-bending force

Table 2 The polarity and mechanical parameters (C_{11}, C_{12}, C_{44}, B_u, Y_0 and C_s) in (10^{11} dyn/cm^2) of AlxIn1−xP at T = 300 K& p = 0 Kbar for different x

x	α_p	C_{11}	C_{12}	C_{44}	B_u	Y_0	C_s
0	0.4181, 0.33[c], 0.41b	9.1078, 10.22a, 9.8919d, 9.3e	3.9745, 4.43c, 4.2941d	3.6633, 4.42a, 3.9874d	5.6856, 5.9e, 7.23a, 6.1601d	6.6928, 6.10a	2.5666, 2.25a, 2.7989d
0.1	0.4118	9.5202	4.1519	3.8302	5.9413	6.9986	2.6842
0.2	0.4034	9.9835	4.3504	4.0179	6.2281	7.3428	2.8165
0.3	0.3930	10.498	4.5702	4.2267	6.5462	7.7257	2.9639
0.4	0.3829	11.030	4.7977	4.4427	6.8753	8.1219	3.1164
0.5	0.3722	11.597	5.0397	4.6727	7.2255	8.5440	3.2788
0.6	0.3609	12.198	5.2959	4.9166	7.5965	8.9914	3.4510
0.7	0.3495	12.828	5.5647	5.1725	7.9858	9.4610	3.6318
0.8	0.3369	13.504	5.8526	5.4473	8.4032	9.9653	3.8259
0.9	0.3245	14.207	6.1519	5.7327	8.8370	10.489	4.0276
1	0.3073, 0.40[c]	15.017, 15.0[a]	6.4956, 6.42[a]	6.0624, 6.11[a]	9.3362, 9.28[a]	11.095, 11.254[e], 11.1[a]	4.2609, 4.421[e], 4.29[a]

[a]Ref. (Ohnuma et al. 2000)

[b]Ref.(Bour et al. 1987)

[c]Ref.(Munns et al. 1993)

[d]Ref.(Keffer et al. 1970)

eRef.(Christian et al. 2013).

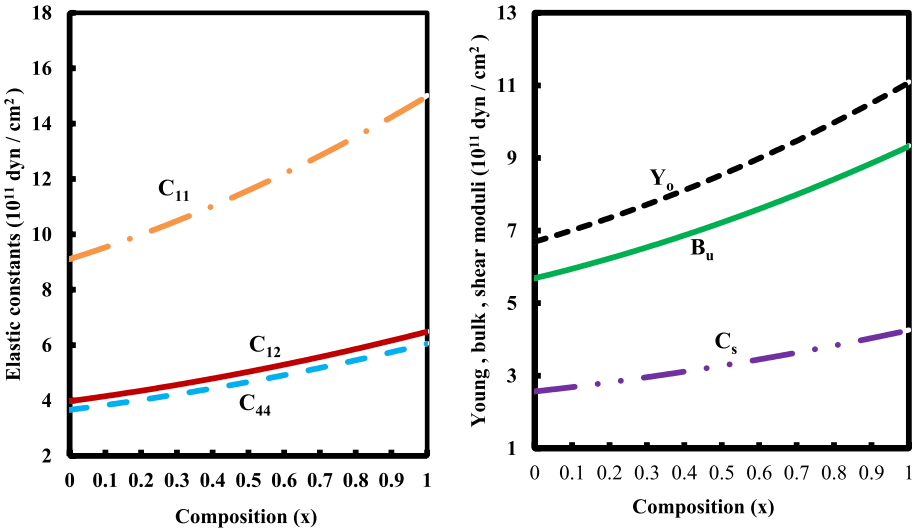

Fig. 3 The mechanical parameters (C_{11}, C_{12}, C_{44}, B_u, Y_0 and C_s) of $Al_xIn_{1-x}P$ as function of Al content at T = 300 K& p = 0 Kbar

parameter (β), internal-strain parameter (ξ), effective charge (Z*) and the transverse effective charge (e_T^*) of $Al_{0.5}In_{0.5}P$ at various values of temperature and pressure are listed in Table 6 and displayed in Fig. 6. Our calculated values of σ, C_0,C_a, B_o, A, α, β, ξ, e_T^* and Z^* of $Al_{0.5}In_{0.5}P$ alloy at the higher values of temperature and pressure may serve as a prediction for future work. This is due to the lack of published data. It was found that every one of these quantities is marginally influenced by temperature. Moreover, with pressure increasing, both α and β increase monotonously, C_0 decreases, while the σ,C_a, B_o, A, ξ, e_T^* and Z^* have weak influence with pressure.

4 Conclusions

Based on (EPM) within VCA, the mechanical properties of zinc-blende $Al_xIn_{1-x}P$ ternary semiconductor alloys were studied under the influence of temperature and pressure. The optoelectronic and mechanical properties of $Al_xIn_{1-x}P$ were successfully determined. All quantities were studied for various estimations of temperature from 0 to 600 K and pressure from 0 to 120 Kbar. Our calculations at p = 0 Kbar and T = 300 K for the AlP and InP were found in excellent accord with the accessible theoretical and experimental data which may be a help for the outcome of the studied ternary alloys. The determined properties in this study may give helpful for optoelectronic applications.

Table 3 The (σ), (C_0), (C_a), (B_0), (A), (α), (β), (ξ), (e_T*) and (Z*) of $Al_xIn_{1-x}P$ at T = 300 K&p = 0 Kbar for various compositions

x	Σ	$C_0(10^{-13})$ (cm^2/dyn)	C_a	B_0	A	α (N/m)	β (N/m)	ξ	e_T*	Z*
0	0.7006, 0.508[a], 0.70[d]	2.1453, 2.13[d], 1.07[a]	1.0850, 1.07[d], 1.3[a]	5.8628, 4.61[a], 5.4[d]	0.3038, 0. 359[a]	30.858, 35.36[h], 33.416[g]	7.5318, 8.42[h], 8.2133[g]	0.6076, 0.595[h], 0.652[e], 0.6054[g]	2.4236, 2.40[f], 2.19[h]	1.5035
0.1	0.7008	2.1443	1.0840	5.6104	0.3037	32.022	7.8223	0.6074	2.4084	1.4965
0.2	0.7010	2.1430	1.0827	5.3521	0.3035	33.331	8.1510	0.6070	2.3878	1.4871
0.3	0.7012	2.1414	1.0813	5.0920	0.3033	34.784	8.5172	0.6066	2.3617	1.4756
0.4	0.7015	2.1400	1.0799	4.8483	0.3031	36.272	8.8922	0.6062	2.3358	1.4644
0.5	0.7017	2.1386	1.0785	4.6133	0.3029	37.845	9.2891	0.6058	2.3076	1.4526
0.6	0.7019	2.1371	1.0771	4.3880	0.3027	39.500	9.7071	0.6055	2.2772	1.4402
0.7	0.7021	2.1358	1.0758	4.1741	0.3025	41.221	10.142	0.6051	2.2458	1.4277
0.8	0.7023	2.1343	1.0744	3.9667	0.3024	43.057	10.606	0.6047	2.2102	1.4138
0.9	0.7026	2.1330	1.0731	3.7720	0.3022	44.945	11.084	0.6043	2.1743	1.4001
1	0.7028, 0.702[a]	2.1312	1.0715, 1.05[a], 1.0836[c]	3.5704, 3.59[a]	0.3019, 0.272[b], 0.3036[c]	47.128, 43.25[h]	11.640, 10.19[h]	0.6039, 0.618[e]	2.1231, 2.38[h]	1.3811

[a]Ref. (Ohnuma et al. 2000)

[b]Ref.(Christian et al. 2013)

[c]Ref. (Tsang and Cohen 1971)

[d]Ref.(Degheidy et al. 2018b)

[e]Ref.(Tan et al. 2010)

[f]Ref.(Bour et al. 1987)

[g]Ref.(Keffer et al. 1970)

[h]Ref.(Munns et al. 1993)

Table 4 The $\left(E_g^L, E_g^\Gamma, \text{and } E_g^X\right)$ in eV of $Al_{0.5}In_{0.5}P$ for different values of temperature and pressure

T(K)							
	0	100	200	300	400	500	600
E_g^L(eV)	3.3349	3.3269	3.3109	3.2871	3.2594	3.2329	3.2144
E_g^Γ(eV)	2.6930	2.6789	2.6592	2.6373	2.5849	2.5397	2.5081
E_g^X(eV)	2.3863	2.3729	2.3582	2.3425	2.3188	2.2880	2.2694
p(Kbar)							
	0	20	40	60	80	100	120
E_g^L(eV)	3.2871	3.2958	3.3340	3.3716	3.4176	3.4546	3.4909
E_g^Γ(eV)	2.6373	2.7330	2.8647	2.9913	3.1070	3.2265	3.3425
E_g^X(eV)	2.3425	2.2880	2.2420	2.2105	2.1713	2.1318	2.0896

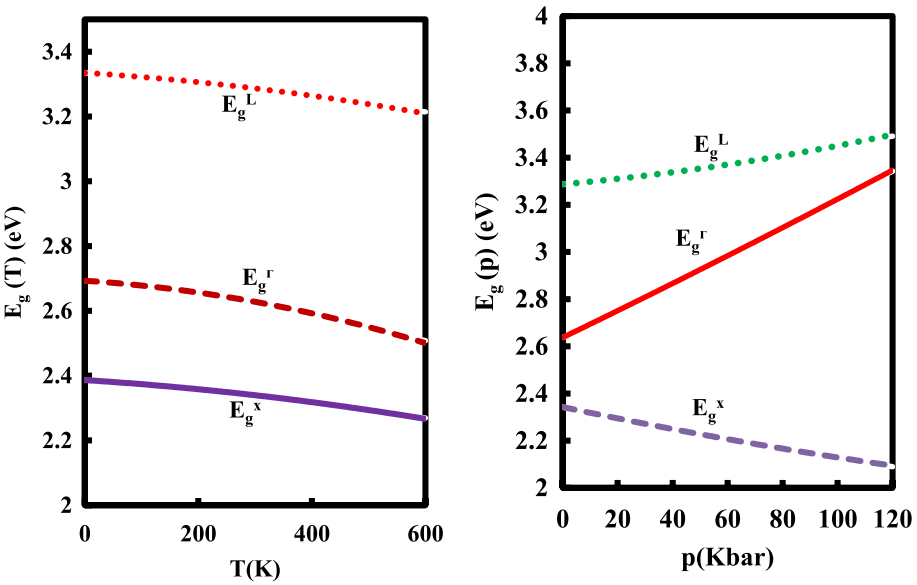

Fig. 4 The energy band gaps of $Al_{0.5}In_{0.5}P$ as function of temperature and pressure

Table 5 Polarity and elastic moduli (C_{11}, C_{12}, C_{44}, B_u, $Y_{0,}$ and C_s) in 10^{11} dyn/cm^2 of $Al_{0.5}In_{0.5}P$ at different values of T and p

	T(K)							P(Kbar)						
	0	100	200	300	400	500	600	0	20	40	60	80	100	120
α_p	0.380	0.377	0.374	0.372	0.372	0.369	0.368	0.372	0.372	0.373	0.373	0.373	0.373	0.373
C_{11}	11.570	11.585	11.597	11.597	11.566	11.578	11.576	11.597	12.083	12.518	12.943	13.345	13.725	14.088
C_{12}	5.031	5.037	5.041	5.040	5.026	5.030	5.028	5.040	5.251	5.440	5.625	5.800	5.965	6.123
C_{44}	4.661	4.667	4.672	4.673	4.660	4.665	4.665	4.673	4.868	5.044	5.215	5.377	5.530	5.676
B_u	7.211	7.220	7.226	7.226	7.206	7.213	7.211	7.226	7.528	7.800	8.064	8.315	8.552	8.778
Y_0	8.520	8.533	8.543	8.544	8.521	8.531	8.530	8.544	8.902	9.222	9.535	9.831	10.111	10.379
C_s	3.269	3.274	3.278	3.279	3.270	3.274	3.274	3.279	3.416	3.539	3.659	3.773	3.880	3.983

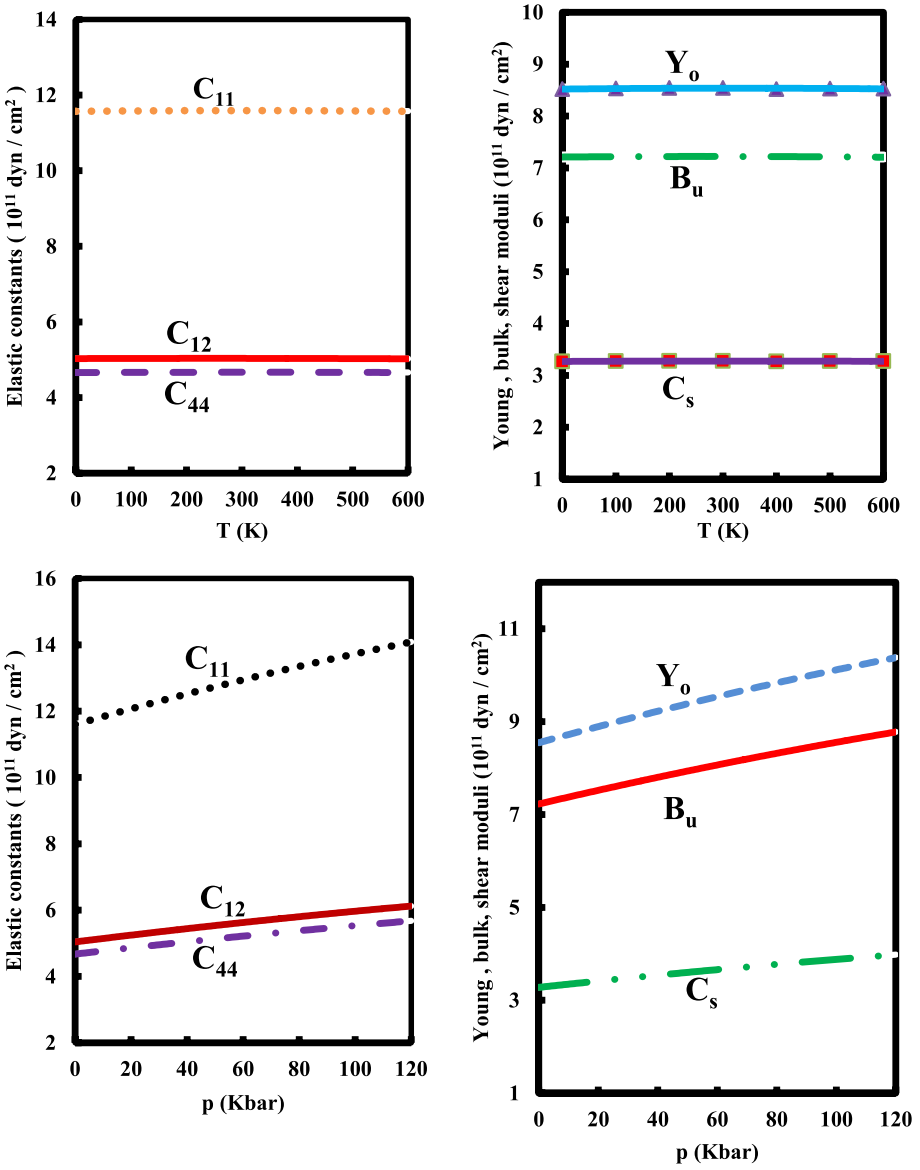

Fig. 5 The elastic moduli (C_{11}, C_{12}, C_{44}, B_u, Y_0 and C_s) of $Al_{0.5}In_{0.5}P$ as function of temperature and pressure

Table 6 The (σ), (C_0), (C_a), (B_0), (A), (α), (β), (ξ), (Z*) and (e_T*) of $Al_{0.5}In_{0.5}P$ alloy at various temperatures and pressures

	T(K)							P(Kbar)						
	0	100	200	300	400	500	600	0	20	40	60	80	100	120
σ	0.3031	0.3030	0.3030	0.3029	0.3029	0.3029	0.3028	0.3029	0.3029	0.3029	0.3029	0.3029	0.3029	0.3029
C_o (10^{-13} cm^2/dyn)	4.6228	4.6171	4.6130	4.6133	4.6259	4.6216	4.6227	4.6133	4.4279	4.2738	4.1336	4.0090	3.8978	3.7975
C_a	1.0795	1.0791	1.0788	1.0785	1.0785	1.0782	1.0779	1.0785	1.0785	1.0786	1.0786	1.0786	1.0786	1.0786
B_0	2.1396	2.1392	2.1388	2.1386	2.1386	2.1382	2.1380	2.1386	2.1386	2.1387	2.1387	2.1387	2.1387	2.1387
A	0.7015	0.7016	0.7016	0.7017	0.7017	0.7017	0.7018	0.7017	0.7017	0.7017	0.7017	0.7017	0.7017	0.7017
N/m))α	37.709	37.774	37.828	37.845	37.762	37.816	37.827	37.845	39.107	40.221	41.309	42.333	43.296	44.209
N/m))β	9.2478	9.2669	9.2829	9.2891	9.2688	9.2849	9.2894	9.2891	9.5990	9.8713	10.138	10.389	10.626	10.850
ξ	0.6061	0.6060	0.6059	0.6058	0.6058	0.6057	0.6057	0.6058	0.6058	0.6059	0.6059	0.6059	0.6059	0.6059
e_T*	2.3279	2.3203	2.3130	2.3076	2.3076	2.3002	2.2951	2.3076	2.3076	2.3103	2.3103	2.3103	2.3103	2.3103
Z*	1.4611	1.4579	1.4548	1.4526	1.4526	1.4495	1.4474	1.4526	1.4526	1.4537	1.4537	1.4537	1.4537	1.4537

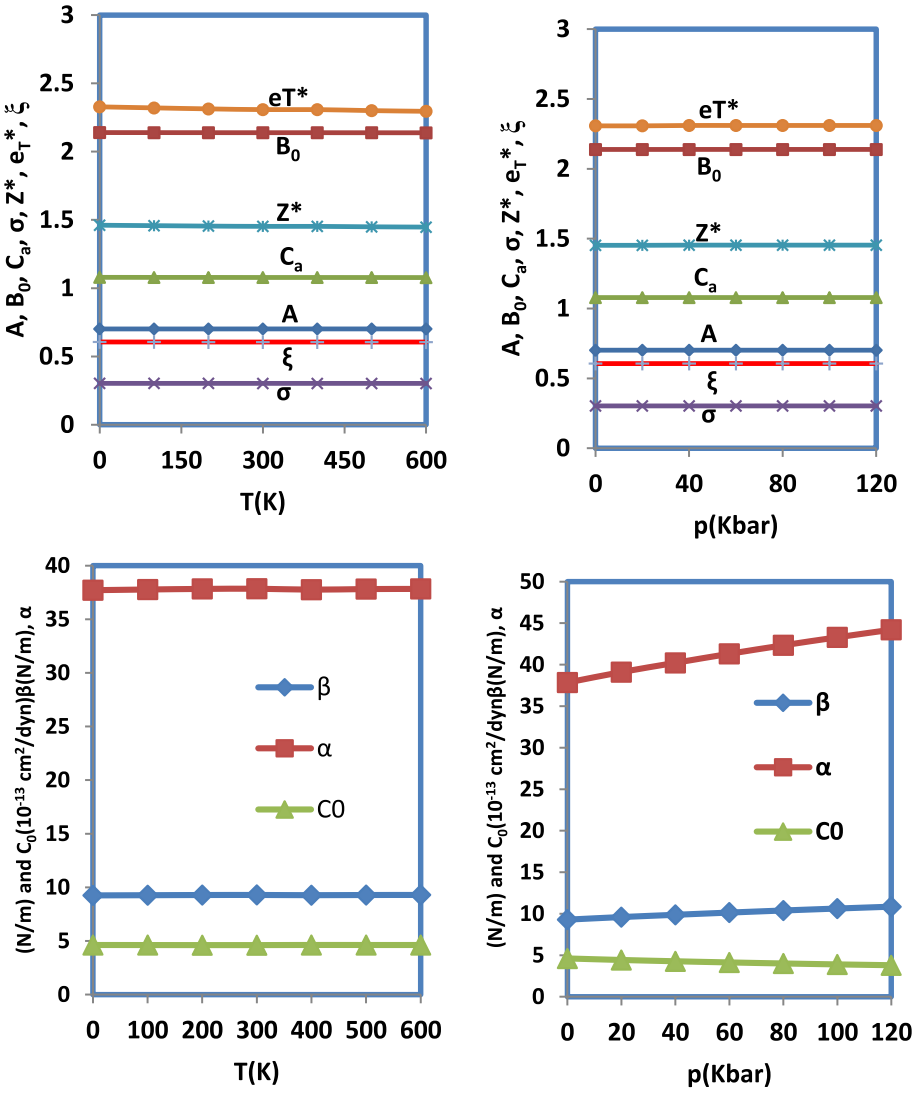

Fig. 6 Mechanical parameters (σ, C_0, C_a, B_o, A, α, β, ξ, e_T^* and Z^*) of $Al_{0.5}In_{0.5}P$ as function of temperature and pressure

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Declarations

Conflict of interest The authors have not disclosed any competing interests.

References

Abdollahi, A., Golzan, M.M., Aghayar, K.: First-Principles Investigation Of Electronic Properties of Al_x In_{1-x} P Semiconductor Alloy. J. Mater. Sci. **51**, 7343–7354 (2016)

Adachi, S.: Band Gaps and Refractive Indices of AlGaAsSb, GaInAsSb, and InPAsSb: Key Properties for a Variety of the 2–4-μm Optoelectronic Device Applications. J. Appl. Phys. **61**, 4869–4876 (1987)

Adachi, S.: Properties of Group-iv, III-v and II-VI Semiconductors. John Wiley, Chichester (2005)

Al Maaitah, I.F., Elkenany, E.B.: Elastic, Lattice Dynamical, Thermal, Electronic, and Optical Properties of Nano-Semiconductor CdTe Under the Effect of Temperature. Comput. Condens. Matter. **30**, e00640 (2022)

Al-Douri, Y., Hashim, U., Khenata, R., Reshak, A.H., Ameri, M., Bouhemadou, A., Ruslinda, A.R., Arshad, M.K.M.: Ab Initio Method of Optical Investigations of CdS_{1-x}Tex Alloys Under Quantum Dots Diameter Effect. Sol. Energy. **115**, 33–39 (2015)

Bouarissa, N.: Compositional Dependence of the Elastic Constants and the Poisson Ratio of GaxIn1− xSb. Mater. Sci. Eng. B. **100**, 280–285 (2003)

Bouarissa, N., Aourag, H.: Conduction Band Edge Charge Densities in $InxGa_{1-x}Sb$. Phys. Status Solidi. **190**, 227–239 (1995)

Bouhemadou, A., Allali, D., Boudiaf, K., Al Qarni, B., Bin-Omran, S., Khenata, R., Al-Douri, Y.: Electronic, Optical, Elastic, Thermoelectric and Thermodynamic Properties of the Spinel Oxides ZnRh2O4 and CdRh2O4. J. Alloys Compd. **774**, 299–314 (2019)

Bour, D.P., Shealy, J.R., Wicks, G.W., Schaff, W.J.: Optical Properties of Al_x In_{1-x} P Grown by Organometallic Vapor Phase Epitaxy. Appl. Phys. Lett. **50**, 615–617 (1987)

Cahn, R.N., Cohen, M.L.: Local Pseudopotential Model for GaSb: Electronic and Optical Properties. Phys. Rev. B. **1**, 2569 (1970)

Chelikowsky, J.R., Cohen, M.L.: Nonlocal Pseudopotential Calculations for the Electronic Structure of Eleven Diamond and Zinc-Blende Semiconductors. Phys. Rev. B. **14**, 556 (1976)

Chen, D., Ravindra, N.M.: Pressure Dependence of Energy Gap of III–V and II–VI Ternary Semiconductors. J. Mater. Sci. **47**, 5735–5742 (2012)

Christian, T.M., Beaton, D.A., Mukherjee, K., Alberi, K., Fitzgerald, E.A., Mascarenhas, A.: Amber-Green Light-Emitting Diodes Using Order-Disorder Al_x In_{1-x} P heterostructures. J. Appl. Phys. **114**, 74505 (2013)

Corkish, R., Green, M.A.: 23rd IEEE Photovoltaic Specialists' Conference, (1993)

Dai, P., Tan, M., Wu, Y.Y., Ji, L., Bian, L.F., Lu, S.L., Yang, H.: Solid-State Tellurium Doping of AlInP and its Application to Photovoltaic Devices Grown by Molecular Beam Epitaxy. J. Cryst. Growth. **413**, 71–75 (2015)

Degheidy, A.R., Elkenany, E.B.: The Response Of Temperature And Hydrostatic Pressure Of Zinc-Blende $GaxIn_{1-x}As$ Semiconducting Alloys. Chinese Phys. B. **21**, 126101 (2012)

Degheidy, A.R., Elkenany, E.B.: Structural and electronic properties of Si_{1-x}Gex binary semiconducting alloys under the effect of temperature and pressure. Semiconductors **47**, 1283–1291 (2013a). https://doi.org/10.1134/S1063782613100084

Degheidy, A.R., Elkenany, E.B.: Electronic and Optical Properties of $InAs_{1-x}Px$ Alloys Under the Effect of Temperature and Pressure. Thin Solid Films **539**, 365–371 (2013b)

Degheidy, A.R., Elkenany, E.B.: Structural and Electronic Properties of Si_{1-x} Ge_x Binary Semiconducting Alloys Under the Effect of Temperature and Pressure. Semiconductors **47**, 1283–1291 (2013c)

Degheidy, A.R., Elkenany, E.B.: Impact of Temperature and Pressure on Mechanical Properties of $GaxIn_{1-x}AsyP_{1-y}$ Alloy Lattice Matched to Different Substrates. J. Alloys Compd. **652**, 379–385 (2015)

Degheidy, A.R., Elkenany, E.B.: Electronic, Optical, and Mechanical Properties of BN, AlN, and InN with zinc-Blende Structure Under Pressure. Chinese Phys. b. **26**, 086103 (2017). https://doi.org/10.1088/1674-1056/26/8/086103

Degheidy, A.R., Elabsy, A.M., Abdelwahed, H.G., Elkenany, E.B.: Pressure Dependence of the Electronic Structure in Ge GaP and InP Semiconductors at Room Temperature. Indian J. Phys. **86**, 363–369 (2012). https://doi.org/10.1007/s12648-012-0059-5

Degheidy, A.R., Elkenany, E.B., Alfrnwani, O.A.: Temperature and Pressure Dependence of Elastic Constants and Related Parameters for InP Semiconductor. Silicon **9**, 183–192 (2017). https://doi.org/10.1007/s12633-016-9408-x

Degheidy, A.R., Elkenany, E.B., Alfrnwani, O.A.: Influence of Composition, Temperature and Pressure on the Optoelectronic and Mechanical Properties of $InPxSb_{1-x}$ Alloys. Comput. Condens. Matter. **16**, e00300 (2018a). https://doi.org/10.1016/j.cocom.2018.e00300

Degheidy, A.R., Elkenany, E.B., Alfrnwani, O.A.: Influence of Composition, Temperature and Pressure on the Optoelectronic and Mechanical Properties of $InPxSb_{1-x}$ Alloys. Comput. Condens. Matter. **16**, e00300 (2018b)

Degheidy, A.R., AbuAli, A.M., Elkenany, E.B.: Phonon Frequencies, Mechanical and Optoelectronic Properties for InP_x As y Sb_{1-x-y}/InAs Alloys Under the Influence of Pressure. Appl. Phys. a. **127**, 1–10 (2021a)

Degheidy, A.R., Alfrnwani, O.A., Elkenany, E.B.: Thermal and Pressure Dependence of Mechanical Properties for $AlxIn_{1-x}PySb_{1-y}$/GaSb System. Bull. Mater. Sci. **44**, 1–8 (2021b)

Elkenany, E.B.: Optoelectronic and Mechanical Properties of InSb Semiconductor Under the Effect of Temperature. Silicon **8**, 391–396 (2016). https://doi.org/10.1007/s12633-015-9317-4

Elkenany, E.B.: High Pressure Dependence of Acoustic Velocities, Phonon Frequencies and Mechanical Properties of $Al_{1-x}InxN$ Ternary Alloys. Phys. Scr. **96**, 105701 (2021a)

Elkenany, E.B.: Acoustic Velocity and Phonon Frequencies of $GaxIn_{1-x}Sb$ Alloys Under Pressure, Temperature, and Compositions. Phys. Scr. **96**, 95701 (2021b)

Elkenany, E.B.: Energy Band Structure, Acoustic Velocities, Optical Phonon Frequencies and Mechanical Properties of $InP_{1-x}Sbx$ Alloys Under Temperature and Pressure. Infrared Phys. Technol. **115**, 103720 (2021c)

Elkenany, E.B., Othman, M.S.H.: Influence of Pressure and Temperature on Mechanical and Thermal Behaviors of InAsSb and GaAsSb Alloys. Phys. Scr. **96**, 125718 (2021)

Fan, H.Y.: Temperature Dependence of the Energy Gap in Semiconductors. Phys. Rev. **82**, 900 (1951)

Ishitani, Y., Hamada, H., Minagawa, S., Yaguchi, H., Shiraki, Y.: The Γc–Γv Transition Energies of $AlxIn_{1-x}P$ Alloys. Jpn. J. Appl. Phys. **36**, 6607 (1997)

Jappor, H.R., Abdulsattar, M.A., Abdul-Lettif, A.M.: Electronic Structure of AlP Under Pressure Using Semiempirical Method. Open Condens. Matter Phys. J. **3**, 1–7 (2010)

Keffer, C., Hayes, T.M., Bienenstock, A.: Debye-Waller Factors and the PbTe Band-gap Temperature Dependence. Phys. Rev. B. **2**, 1966–1976 (1970)

Lee, S.J., Kwon, T.S., Nahm, K., Kim, C.K.: Band Structure of Ternary Compound Semiconductors Beyond the Virtual Crystal Approximation. J. Phys. Condens. Matter. **2**, 3253–32557 (1990)

Lin, C. C., Chen, K. J., Lin, D.-W., Han, H.-V., Lai, W.C., Huang, J.J., Lu, T.C., Chang, S.J., Kuo, H.C.: Light Emitting Diodes. In: Lee, C.C. (ed.) The Current Trends of Optics and Photonics, pp. 179–234. Springer, Berlin (2015)

Mezrag, F., Bouarissa, N.: Optical Properties of $AlxIn_{1-x}P$ Ternary Semiconductor Alloys. J. Comput. Methods Sci. Eng. **18**, 299–305 (2018)

Moakafi, M., Khenata, R., Bouhemadou, A., Khachai, H., Amrani, B., Rached, D., Rérat, M.: Electronic and Optical Properties Under Pressure Effect of Alkali Metal Oxides. Eur. Phys. J. B. **64**, 35–42 (2008)

Moss, T.S.: A Relationship Between the Refractive Index and the Infra-Red Threshold of Sensitivity for Photoconductors. Proc. Phys. Soc. Sect. B. **63**, 167–176 (1950)

Munns, G.O., Chen, W.L., Sherwin, M.E., Haddad, G.I.: The Growth of InAlP Using Trimethyl Amine Alane by Chemical Beam Epitaxy. J. Cryst. Growth. **127**, 226–229 (1993)

Ohnuma, T., Nagano, M., Nemoto, K.: Indirect-to-Direct Transition of (AlAs) n/(AlP) n Strained Short-Period Superlattices. Jpn. J. Appl. Phys. **39**, L972–L974 (2000)

Ouahrani, T., Otero-de-la-Roza, A., Reshak, A.H., Khenata, R., Faraoun, H.I., Amrani, B., Mebrouki, M., Luaña, V.: Elastic Properties and Bonding of the $AgGaSe_2$ Chalcopyrite. Phys. B Condens. Matter. **405**, 3658–3664 (2010)

Pandey, K.C., Phillips, J.C.: Nonlocal Pseudopotentials for Ge and GaAs. Phys. Rev. B. **9**, 1552 (1974)

Phillips, J.C., Pandey, K.C.: Nonlocal Pseudopotential for Ge. Phys. Rev. Lett. **30**, 787 (1973)

Reshak, A.H., Kityk, I.V., Khenata, R., Auluck, S.: Effect of Increasing Tellurium Content on the Electronic and Optical Properties of Cadmium Selenide Telluride Alloys $CdSe_{1-x}Tex$: An ab Initio Study. J. Alloys Compd. **509**, 6737–6750 (2011)

Saib, S., Bouarissa, N., Rodríguez-Hernández, P., Muñoz, A.: Structural and Dielectric Properties of AlN Under Pressure. Phys. B Condens. Matter. **403**, 4059–4062 (2008)

Samara, G.A.: Temperature and Pressure Dependences of the Dielectric Constants of Semiconductors. Phys. Rev. B. **27**, 3494–3505 (1983)
Shen, S.-G.: Calculation of the Elastic Properties of Semiconductors. J. Phys. Condens. Matter. **6**, 8733–8743 (1994)
Skelton, E.F., Radoff, P.L., Bolsaitis, P., Verbalis, A.: Mean-Square Atomic Displacements in HgTe and Their Temperature Dependence. Phys. Rev. B. **5**, 3008 (1972)
Tan, J., Ji, G., Chen, X., Zhang, L., Wen, Y.: The High-Pressure Phase Transitions and Vibrational Properties of Zinc-Blende XTe (X= Zn, Cd, Hg): Performance of Local-Density-Approximation Density Functional Theory. Comput. Mater. Sci. **48**, 796–801 (2010)
Tiwari, S., Frank, D.J.: Empirical Fit to Band Discontinuities and Barrier Heights in III–V alloy Systems. Appl. Phys. Lett. **60**, 630–632 (1992)
Tsang, Y.W., Cohen, M.L.: Calculation of the Temperature Dependence of the Energy Gaps in PbTe and SnTe. Phys. Rev. B. **3**, 1254–1261 (1971)
Tukiainen, A., Toikkanen, L., Haavisto, M., Erojarvi, V., Rimpilainen, V., Viheriala, J., Pessa, M.: AlInP–AlGaInP Quantum-Well Lasers Grown by Molecular Beam Epitaxy. IEEE Photonics Technol. Lett. **18**, 2257–2259 (2006)
Vegard, L.: Die konstitution der Mischkristalle Und Die Raumfüllung Der Atome. Zeitschrift Für Phys. **5**, 17–26 (1921)
Vogl, P.: Dynamical Effective Charges in Semiconductors: A Pseudopotential Approach. J. Phys. C Solid State Phys. **11**, 251–262 (1978)
Vurgaftman, I., áR Meyer, J., áR Ram-Mohan, L.: Band Parameters for III–V Compound Semiconductors and Their Alloys. J. Appl. Phys. **89**, 5815–5875 (2001)
Walter, J.P., Cohen, M.L.: Calculation of the Reflectivity, Modulated Reflectivity, and Band Structure of GaAs, GaP, ZnSe, and ZnS. Phys. Rev. **183**, 763–772 (1969)
Walter, J.P., Cohen, M.L.: Wave-Vector-Dependent Dielectric Function for Si, Ge, GaAs, and ZnSe. Phys. Rev. B. **2**, 1821–1826 (1970)
Wang, H.Y., Cao, J., Huang, X.Y., Huang, J.M.: Pressure Dependence of Elastic and Dynamical Properties of Zinc-Blende ZnS and ZnSe From First Principle Calculation. arXiv Prepr. arXiv1204.6102. (2012)
Zhang, Y.-G., Li, C., Gu, Y., Wang, K., Li, H., Shao, X.-M., Fang, J.-X.: GaInP–AlInP–GaAs Blue Photovoltaic Detectors with Narrow Response Wavelength Width. IEEE Photonics Technol. Lett. **22**, 944–946 (2010)