Electronic, optical, and mechanical properties of AlₓIn₁₋ₓP alloys under temperature and pressure

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Abstract
In this work, the optoelectronic and mechanical properties of AlₓIn₁₋ₓP combinations in the zinc-blende structure were studied for different Al concentrations. The energy band gaps \( E_{g} \), \( E_{\Gamma} \), \( E_{X} \), refractive index (n), high frequency and static dielectric constants (\( \varepsilon_{\infty} \), \( \varepsilon_{0} \)), elastic parameters \( (C_{11}, C_{12}, C_{44}) \) were investigated. Other mechanical properties such as bulk \( (B_{b}) \), shear \( (C_{s}) \), Young’s \( (Y_{0}) \) moduli, Poisson ratio (\( \sigma \)), linear compressibility \( (C_{v}) \), Cauchy \( (C_{a}) \) ratio, isotropy factor \( (A) \), bond stretching parameter \( (\alpha) \), bond-bending force parameter \( (\beta) \), internal-strain parameter \( (\xi) \), 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 AlₓIn₁₋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
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_{x}In_{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_{x}In_{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 semiconductor alloys, 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 Ravinda 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 \( E^L_g, E^F_g, E^X_g \), optical properties such as refractive index, dielectric constants \( n, \varepsilon_\infty, \varepsilon_0 \) and mechanical properties such as elastic constants \( C_{11}, C_{12}, C_{44} \), bulk, shear and Young’s moduli \( B_\omega, C_s, Y_0 \) for Al_{x}In_{1-x}P alloys have been calculated. The Poisson ratio \( \sigma \), linear compressibility \( C_\rho \), Cauchy ratio \( C_\mu \), anisotropy factor \( A \), bond stretching parameter \( \alpha \), bond-bending force parameter \( \beta \), internal-strain parameter \( \xi \), and the transverse effective charge \( e^T_T \) for Al_{x}In_{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_{x}In_{1-x}P ternary alloys.

2 Theory and calculations

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

\[
V(r)_{\text{alloy}} = V_{\text{VCA}}(r) + V_{\text{dis}}(r)
\]

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

\[ V_{\text{VCA}}(r) = x V_{\text{AlP}}(r) + (1-x) V_{\text{InP}}(r) \]  

(2)

\[ V_{\text{dis}}(r) = -\Omega \sqrt{x(1-x)} [V_{\text{AlP}}(r) - V_{\text{InP}}(r)] \]  

(3)

where \( x \) is the Aluminum concentration (Al) and \( \Omega \) 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

\[ W_{S, A} = x W_{S, A}^{\text{AlP}} + (1-x) W_{S, A}^{\text{InP}} - \sqrt{x(1-x)} [W_{S, A}^{\text{AlP}} - W_{S, A}^{\text{InP}}] \]  

(4)

where \( W_{S, A}^{\text{AlP}}, W_{S, A}^{\text{InP}} \) are the symmetric and anti-symmetric form factors of the AlP and InP, respectively. The lattice constant of \( \text{Al}_x\text{In}_{1-x}\text{P} \) alloy was acquired by the Vegard’s relation (Vegard 1921)

\[ a_{\text{alloy}} = (1-x) a_{\text{InP}} + x a_{\text{AlP}} \]  

(5)

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

\[ \left\| \frac{1}{2} \left( \tilde{k} + \tilde{G}' \right) \right\|^2 - E_{nk} + \sum_{\tilde{G} \neq \tilde{G}'} V(\left\{ \tilde{G}' \right\}) = 0 \]  

(6)

where

\[ V(\left\{ \tilde{G}' \right\}) = W^S(\Delta \tilde{G}) \cos(\Delta \tilde{G} \cdot \vec{\tau}) + i W^A(\Delta \tilde{G}, x) \sin(\Delta \tilde{G} \cdot \vec{\tau}) \]

is the pseudo-potential and \( \vec{\tau} \) is the atomic position and equals to \( \frac{a}{8}(1, 1, 1) \). The calculated values of the fundamental energy band gaps of \( \text{Al}_x\text{In}_{1-x}\text{P} \) alloy were utilized to determine \( n \) (Moss 1950) and the \( \varepsilon_\infty \) by applying the Samara relation (Samara 1983). The gained \( W^S \) and \( W^A \) at \( G(1,1,1) \) were utilized to determine the \( \alpha_p \) using Vogl’s relation (Vogl 1978) as

\[ \alpha_p = -\frac{w^A_3}{w^S_3} \]  

(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 \( B_\alpha, C_\alpha, \) and \( Y_\sigma \) of \( \text{Al}_x\text{In}_{1-x}\text{P} \) alloys (Cahn and Cohen 1970; Pandey and Phillips 1974; Walter and Cohen 1969). Other significant parameters as the ratio \( \sigma, C_{\alpha}, C_\sigma, \) and \( A \) were also successfully calculated (Bouarissa 2003; Shen 1994). Finally, the \( \alpha, \beta, \xi \) and \( e_\tau^* \) 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 \( E_{\text{g}}^{L} \), \( E_{\text{g}}^{\Gamma} \), \( E_{\text{g}}^{X} \) with Al content in Al\(_{x}\)In\(_{1-x}\)P is recorded in Table 1 and shown in Fig. 1. It was seen that \( E_{\text{g}}^{L} \) and \( E_{\text{g}}^{\Gamma} \) are raised with different rates with increasing Al content, however, \( E_{\text{g}}^{X} \) is increased with a weaker rate. We noted that Al\(_{x}\)In\(_{1-x}\)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\(_{x}\)In\(_{1-x}\)P introduced the optical bowing parameters as \(-1.6\) eV, \(-0.49\) eV, and \(0.27\) eV at L, \(\Gamma\), 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 \( E_{\text{g}}^{L} \), \( E_{\text{g}}^{\Gamma} \), \( E_{\text{g}}^{X} \) 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:

\[
E_{\text{g}}^{L} = 2.0552 + 3.2277x - 1.6015x^2
\]

\[
E_{\text{g}}^{\Gamma} = 1.358 + 2.7848x - 0.4931x^2
\]

| x    | \( E_{\text{g}}^{L}\) (eV) | \( E_{\text{g}}^{\Gamma}\) (eV) | \( E_{\text{g}}^{X}\) (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\(^{c}\) | 2.5460, 2.4878\(^{c}\), 2.5\(^{c}\), 2.45\(^{d}\), 2.52\(^{c}\) |

\(^{a}\)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)
Figure 2 displays the variation of refractive index (n), optical and static dielectric constants ($\varepsilon_\infty$, $\varepsilon_0$) of $\text{Al}_x\text{In}_{1-x}\text{P}$ with composition at $T = 300$ K and $p = 0$ Kbar. It was seen that

$$E_g^X = 2.2421 + 0.0438x + 0.2742x^2$$

Figure 2 displays the variation of refractive index (n), optical and static dielectric constants ($\varepsilon_\infty$, $\varepsilon_0$) of $\text{Al}_x\text{In}_{1-x}\text{P}$ with composition at $T = 300$ K and $p = 0$ Kbar. It was seen that
the refractive index is slightly linear decreased with enhancing composition. It was also found that the optical and static dielectric constants \((\varepsilon_{\infty}, \varepsilon_0)\) 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 \(\alpha_p, C_{11}, C_{12}, C_{44}, B_u, C_s,\) and \(Y_0\) of \(\text{Al}_x\text{In}_{1-x}\text{P}\) 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 \((C_{11}, C_{12}, \text{and } C_{44})\) 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 \((\sigma)\), linear compressibility \((C_o)\), Cauchy \((C_a)\) ratio, Born ratio \((B_0)\), anisotropy factor \((A)\), bond stretching parameter \((\beta)\), internal-strain parameter \((\xi)\), the transverse effective charge \((\xi_T^*)\), and effective charge \((Z^*)\) of \(\text{Al}_x\text{In}_{1-x}\text{P}\) 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 \(\alpha\) and \(\beta\) 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 \(\text{Al}_x\text{In}_{1-x}\text{P}\) alloy.

### 3.2 Influence of pressure and temperature

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

The determined polarities \(\alpha_p, C_{11}, C_{12}, C_{44}, B_u, C_s,\) and \(Y_0\) of \(\text{Al}_{0.5}\text{In}_{0.5}\text{P}\) 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 \(Y_0\) of \(\text{Al}_{0.5}\text{In}_{0.5}\text{P}\) 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 \((0–600 \text{ K})\) and pressures from \((0–120 \text{ Kbar})\) which indicates the stability of \(\text{Al}_x\text{In}_{1-x}\text{P}\) in its structure.

The calculated Poisson ratio \((\sigma)\), linear compressibility \((C_0)\), Cauchy ratio \((C_a)\), Born ratio \((B_0)\), anisotropy factor \((A)\), bond stretching parameter \((\alpha)\), 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 Al$_x$In$_{1-x}$P at $T = 300$ K & $p = 0$ Kbar for different $x$

| $x$ | $\alpha_p$ | $C_{11}$ | $C_{12}$ | $C_{44}$ | $B_u$ | $Y_0$ | $C_s$ |
|-----|-------------|----------|----------|----------|-------|-------|-------|
| 0   | 0.4181, 0.33$^c$, 0.41$^b$ | 9.1078, 10.22$^a$, 9.8919$d$, 9.3$^e$ | 3.9745, 4.43$c$, 4.2941$d$ | 3.6633, 4.42$a$, 3.9874$d$ | 5.6856, 5.9$^e$, 6.6928, 6.10$a$ | 2.5666, 2.25$a$, 2.7989$d$ |
| 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 | 2.9165 |
| 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 | 9.7653 | 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$^c$, 11.1$^a$ | 4.2609, 4.421$^c$, 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)
$^e$Ref. (Christian et al. 2013).
parameter ($\beta$), internal-strain parameter ($\xi$), 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 $\sigma$, $C_0$, $C_a$, $B_o$, $A$, $\alpha$, $\beta$, $\xi$, $e^*_T$ 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 $\alpha$ and $\beta$ increase monotonously, $C_0$ decreases, while the $\sigma$, $C_a$, $B_o$, $A$, $\xi$, $e^*_T$ and $Z^*$ have weak influence with pressure.

### 4 Conclusions

Based on (EPM) within VCA, the mechanical properties of zinc-blende Al$_x$In$_{1-x}$P ternary semiconductor alloys were studied under the influence of temperature and pressure. The optoelectronic and mechanical properties of Al$_x$In$_{1-x}$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), (C₀), (Cₐ), (B₀), (A), (α), (β), (ξ), (e₆*) and (Z*) of AlₓIn₁₋ₓP at T = 300 K & p = 0 Kbar for various compositions

| x  | Σ     | C₀(10⁻¹³) (cm²/dyn) | Cₐ  | B₀     | A      | α (N/m) | β (N/m) | ξ      | e₆*    | Z*     |
|----|-------|---------------------|------|--------|--------|---------|---------|--------|--------|--------|
| 0  | 0.7006, 0.508ₐ, 0.70ₐ | 2.1453, 2.13ₐ | 1.0850, 1.07ₐ, 1.3ₐ | 5.862ₐ, 4.61ₐ, 5.4ₐ | 0.303ₐ, 0.359ₐ | 30.85ₐ, 35.3ₐ | 7.5ₐ, 8.4₂ₐ, 8.2₁₃ₐ | 0.6ₐ, 0.5ₐ, 0.5ₐ | 2.4₂₃ₐ, 2.4₀₁₉ₐ | 1.₅₀₃ₐ |
| 0.1 | 0.700ₐ | 2.₁₄₄₃ | 1.₀₈₄₀ | 5.₆₁₀₄ | 0.₃₀₃ₗ | 3₂.₀₂₄ | 7.₈₂₃ₗ | 0.₆₀₇₄ | 2.₄₀₈₄ | 1.₄₉₆₅ |
| 0.2 | 0.70₁₀ | 2.₁₄₃₀ | 1.₀₈₂ₗ | 5.₅₃₂₁ | 0.₃₀₃ₗ | 3₃.₃₁₃ | 8.₁₅₁₀ | 0.₆₀₇₀ | 2.₃₇₈ₗ | 1.₄₈₇₁ |
| 0.3 | 0.70₁₂ | 2.₁₄₁₄ | 1.₀₈₁₃ | 5.₀₉₂₀ | 0.₃₀₃ₗ | 3₄.₇₈₄ | 8.₅₁₇₂ | 0.₆₀₆₆ | 2.₃₆₁₇ | 1.₄₇₅₆ |
| 0.4 | 0.70₁₅ | 2.₁₄₀₀ | 1.₀₇₉₉ | 4.₈₄₈₃ | 0.₃₀₃ₗ | 3₆.₂₇₃ | ₈.₉₉₂₂ | 0.₆₀₆₂ | 2.₃₃₅₈ | 1.₄₆₄₄ |
| 0.5 | 0.70₁₇ | 2.₁₃₈₆ | 1.₀₇₈₅ | 4.₆₁₃₃ | 0.₃₀₂₉ | 3₇.₈₄₅ | ₉.₈₉₁₁ | 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 | ₁₀.₆₆₆ | 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, 0.70₂ₐ | 2.₁₃₁₂ | 1.₀₇₁₅, 1.₀₅₄₇, 1.₀₈₃₆ₐ | ₃.₅₇₀₄, ₃.₅₉ₐ | ₀.₃₀₁₉, ₀.₂₇₂ₐ, ₀.₃₀₃ₐ | ₄₇.₁₂₈, ₄₃.₂₅₈ | ₁₁.₆₄₀, ₁₀.₁₉₈ | ₀.₆₀₃₉, ₀.₆₁₈ | ₂.₁₂₃₁, ₂.₃₈₉ | ₁.₃₈₁₁ |

ₐRef. (Ohnuma et al. 2000)
₉Ref. (Christian et al. 2013)
ₐRef. (Tsang and Cohen 1971)
ₐRef. (Degheidy et al. 2018b)
ₐRef. (Tan et al. 2010)
ₐRef. (Bour et al. 1987)
ₐRef. (Keffer et al. 1976)
ₐRef. (Munns et al. 1993)
Table 4 The \( E^L_g, E^Γ_g, \) and \( E^X_g \) 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 |
|-------|-----|-----|-----|-----|-----|-----|-----|
| \( E^L_g \) (eV) | 3.3349 | 3.3269 | 3.3109 | 3.2871 | 3.2594 | 3.2329 | 3.2144 |
| \( E^Γ_g \) (eV) | 2.6930 | 2.6789 | 2.6592 | 2.6373 | 2.5849 | 2.5397 | 2.5081 |
| \( E^X_g \) (eV) | 2.3863 | 2.3729 | 2.3582 | 2.3425 | 2.3188 | 2.2880 | 2.2694 |
| p(Kbar) |     |     |     |     |     |     |     |
| \( E^L_g \) (eV) | 3.2871 | 3.2958 | 3.3340 | 3.3716 | 3.4176 | 3.4546 | 3.4909 |
| \( E^Γ_g \) (eV) | 2.6373 | 2.7330 | 2.8647 | 2.9913 | 3.1070 | 3.2265 | 3.3425 |
| \( E^X_g \) (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 (C₁₁, C₁₂, C₄₄, Bₜ, Y₀, and C₈) in 10¹¹ dyn/cm² of Al₀.5In₀.5P 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  |
| αₚ     | 0.380   | 0.377| 0.374| 0.372| 0.372| 0.369| 0.368|
| C₁₁    | 11.570  | 11.585| 11.597| 11.597| 11.566| 11.578| 11.576|
| C₁₂    | 5.031   | 5.037| 5.041| 5.040| 5.026| 5.030| 5.028|
| C₄₄    | 4.661   | 4.667| 4.672| 4.673| 4.660| 4.665| 4.665|
| Bₜ     | 7.211   | 7.220| 7.226| 7.226| 7.206| 7.213| 7.211|
| Y₀     | 8.520   | 8.533| 8.543| 8.544| 8.521| 8.531| 8.530|
| C₈     | 3.269   | 3.274| 3.278| 3.279| 3.270| 3.274| 3.274|
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), (C₀), (Cₐ), (B₀), (A), (α), (β), (ξ), (Z*) and (eₜ*) of Al₀.₅In₀.₅P 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 | 0.3029 | 0.3029 | 0.3028 | 0.3029 | 0.3029 | 0.3029 | 0.3029 | 0.3029 |
| C₀(10⁻¹³ cm²/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 |
| Cₐ   | 1.0795 | 1.0791 | 1.0788 | 1.0785 | 1.0785 | 1.0782 | 1.0779 | 1.0785 | 1.0786 | 1.0786 | 1.0786 | 1.0786 | 1.0786 | 1.0786 |
| B₀   | 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 | 0.7017 | 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 | 9.2849 | 9.2894 | 9.2891 | 9.2891 | 9.5990 | 10.138 | 10.389 | 10.626 | 10.850 | 10.850 |
| ξ    | 0.6061 | 0.6060 | 0.6059 | 0.6058 | 0.6058 | 0.6057 | 0.6057 | 0.6058 | 0.6059 | 0.6059 | 0.6055 | 0.6059 | 0.6059 | 0.6059 |
| eₜ*  | 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 ($\sigma, C_0, C_a, B_0, A, \alpha, \beta, \xi, e_T^*$ 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.

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