

## Mechanical and Piezoelectric Properties, Sound Velocity and Debye Temperature of Thallium-Phosphide under Pressure

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**Abstract:** *In the present work, we report a pseudopotential plane wave method (PP-PW) based on density functional theory (DFT) and density functional perturbation theory (DFPT) to study some physical properties of (B3) thallium - phosphide (TIP) compound under hydrostatic pressure. The phase transition pressure, elastic constants, bulk modulus, the direct and converse piezoelectric coefficients, the longitudinal, transverse, and average sound velocities, and finally the Debye temperature under hydrostatic pressure are studied. Our investigation of several quantities under pressure of this compound is up to 12GPa. By analyzing the Poisson's ratio  $\nu$  and the ratio  $R_{G/B}$ , we estimate the critical value of pressure which separates ductile and brittle natures. The melting temperature and the Grüneisen parameter at equilibrium lattice parameter are also obtained. Detailed comparisons with other theoretical data (due to the unavailability of experimental data) reveal good agreement concerning the majority of quantities and discrepancies for some others.*

**Keywords:** *PP-PW method, elastic properties, TIP compound, sound velocity, Debye temperature.*

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### 1. INTRODUCTION

Semiconductor materials (silicon, germanium, selenium; lead telluride; lead sulfide, silicon carbide... etc) have a number of interesting properties, and they are usually used to fabricate and elaborate the majority of electronic devices: modulators, detectors,... etc.

In view of the possibility for eventual technological applications, Thallium - V compounds have attracted increasing theoretical research interest in the last few years. Unfortunately, to our knowledge, they have not been synthesized yet and only a few theoretical works [1-8] of the literature are available. The majority of III-V semiconductor compounds crystallize in zinc-blende (B3) and wurtzite (B4) structures; and generally with very small difference in the total energies of the two phases [6].

Using the plane-wave pseudopotential approach in the framework of density-functional theory within the local density approximation implemented in ABINIT code, Elastic properties and phase stability of 25 III-V binary compounds of both ZB and WZ poly-types have been studied by Wang, H.Q. Ye [1]. The structural parameters, electronic behavior and thermodynamic properties of thallium - phosphide (TIP) in its zincblende phase have been studied by Ciftci et al [4] using the plane-wave pseudopotential approach in the framework of density-functional theory within the LDA and GGA approximations implemented in VASP code.

Under hydrostatic pressure the low pressure phase is destabilized and structural phase transition occurs. For thallium - phosphide compound, the phase transition from zincblende (B3) phase to Rock-salt (B1) phase appears at a range pressure 4.47 GPa to 7.626 GPa [4-7].

In the present work, we report first principle calculations of the hydrostatic pressure effect on : the structural stability, the independent elastic constants, the direct and converse piezoelectric coefficients, the longitudinal, transverse and average sound velocities sound velocities, and finally

the Debye temperature of TIP compound in its structure (B3) phase using the pseudopotential plane wave method in the framework of density functional theory, and the density functional perturbation theory, within the local density approximation. The critical value of pressure which separates ductile and brittle nature, the mechanical stability criteria, the melting temperature and the Grüneisen parameter at equilibrium lattice parameter of this material are also obtained.

## 2. COMPUTATIONAL METHODS

The density-functional theory (DFT) and the density-functional perturbation theory (DFPT) have become a powerful tool for investigating the elastic and mechanical properties of semiconductor materials (in the limit of zero temperature and in the absence of zero-point motion) [9]. For a given crystal it is possible to calculate the complete set of elastic constants by applying small strains to the equilibrium unit cell and determining the corresponding variations in the total energy [9]. The elastic constants and piezoelectric coefficients obtained in the present were carried out using the ABINIT code [10-12] based on the plane-wave pseudopotential approach in the framework of the DFT and DFPT. ABINIT code is a package whose main program allows one to find the total energy and several others properties of systems within density functional theory, using pseudopotentials and a plane-wave basis-set. It is a common project of the Université Catholique de Louvain, Corning Incorporated, the Université de Liège, and other contributors.

The Hartwigsen-Goedecker-Hutter (HGH) relativistic separable dual-space Gaussian pseudopotentials [13] in the context of the local density approximation are employed in the computation. The electron-electron interaction was considered within the local density approximation (LDA) by Teter-Pade parameterization [14], which reproduces the correlation scheme of Perdew and Wang [15].

The two parameters that affect considerably the accuracy of calculations are the kinetic energy cutoff and the number of special  $k$ -points used for the Brillouin zone (BZ) integration. The valence electronic wave functions are expanded by a plane-wave basis set with an energy cutoff of 90 Hartree. Integrations in the Brillouin zone are performed using special  $k$ -points generated with  $8 \times 8 \times 8$  Monkhorst-pack meshes [16]. These parameters have been carefully tested to ensure that they lead to well-converged total energy and geometrical configurations.

The elastic stiffness constants and piezoelectric coefficients reported in this article are obtained by the method used in our previous work [17] (for more detail, please visit the website: [http://www.abinit.org/documentation/helpfiles/for-v7.8/tutorial/lesson\\_elastic.html](http://www.abinit.org/documentation/helpfiles/for-v7.8/tutorial/lesson_elastic.html)).

## 3. RESULTS AND DISCUSSIONS

### 3.1. Pressure of the Phase Transition

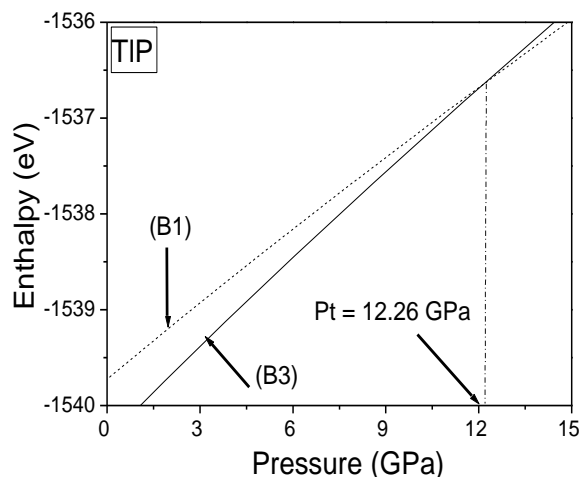
If the hydrostatic pressure is applied on any semiconductor material, this later undergoes structural transformations. Many semiconductor compounds transform from the zincblende phase structure to the site-ordered NaCl (rock salt) structure under pressure [18]. The stability of any particular structure is corresponds by the lowest Gibbs energy, which is given as [19]

$$G = U + PV - TS \quad (1)$$

Where:  $U$  is the total internal energy,  $P$  the pressure,  $V$  the volume,  $T$  the temperature and  $S$  is the entropy.

To investigate the structural transition under hydrostatic pressure, we have optimized (at  $T = 0K$ ) both the cell parameters and atomic positions for zincblende and the NaCl phases under each hydrostatic pressure.

In Fig. 1 we show schematic enthalpy-pressure  $H = H(p)$  curve for two phases (zincblende and the rock salt) of thallium - phosphide material. The two  $H(p)$  curves for phases zincblende and the site-ordered NaCl cross at the pressure  $P_t$  (B3/B1).



**Fig 1.** Enthalpies versus pressure curves of both (B3) and (B1) phases of TIP compound

The phase transition occurs at pressures of 12.26 GPa. This value is presented in table 1, and compared with the available theoretical data [4-7]. It's much higher than the different values of the literature obtained from first principle calculations [4, 5], and from the Interaction Potential Model (IPM) [6].

**Table 1.** Phase transition pressure (in GPa) from (B3) TIP to (B1) TIP in comparison with the available theoretical data [4-7].

Parameter	Our work	Other works			
Pt (GPa)	12.26	4.47[4]LDA	7.29[5]GGA	7.2[6]IPM	7.626[7]

### 3.2. Elastic Constants and The Bulk Modulus

The number of elastic constants, that characterize the material, is usually reduced if the crystal possesses symmetry elements, and in the case of cubic crystals there are only three independent constants ( $C_{11}$ ,  $C_{12}$  and  $C_{44}$ ). For cubic crystals, the bulk modulus  $B$  and the elastic constants ( $C_{11}$  and  $C_{12}$ ) are related by:

$$B = (C_{11} + 2C_{12})/3 \quad (2)$$

The evaluated elastic constants  $C_{ij}$  and the bulk modulus  $B$  of (B3) TIP at zero-pressure are presented in table 2, and compared with the available theoretical data [1, 4-6, 20, 21]. Generally, we notice a good agreement between the elastic constants ( $C_{12}$  and  $C_{44}$ ) and previous theoretical values [1, 4-6, 20, 21].

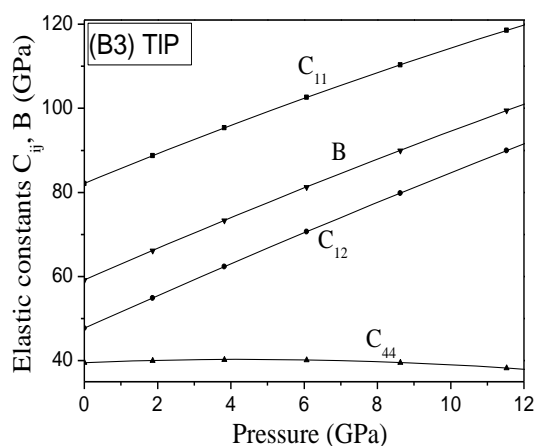
**Table 2.** Elastic constants  $C_{ij}$  and bulk modulus  $B$  in (GPa) in comparison with other theoretical data [1, 4-6, 20, 21]. <sup>a</sup> from the relation  $B = V \frac{\partial^2 E}{\partial V^2}$ , <sup>b</sup> from the relation  $B = (C_{11} + 2C_{12})/3$

Parameter	Our work	Other works			
$C_{11}$	82.15	107.6[1]LDA	94.63[4]	75.53[5]GGA	117.85[6]
$C_{12}$	47.71	53.2[1]LDA	50.75[4]	39.79[5]GGA	61.77[6]
$C_{44}$	39.54	53.6[1]LDA	38.55[4]	38.77[5]GGA	88.4[6]
$B$	59.19	46.75[3] GGA	57.536[4] LDA	45.975[4]GGA	53.3[5] <sup>a</sup>
		51.70[5] <sup>b</sup>	80.46[6]	71.30[20]LDA	57[21]LDA

Contrary to ( $C_{12}$  and  $C_{44}$ ), it is clear that our calculated elastic constant  $C_{11}$  is relatively lower than the values obtained by the previously calculated data [1, 4-6], it deviates from the calculated [1] LDA and [4]LDA values with 23.65% and 13.19% respectively. Moreover, we note that the elastic constants calculated in the present work within LDA are relatively large compared to other previously GGA calculated values [5], due to the fact that LDA gives a comparatively smaller lattice constant and a larger bulk modulus than GGA.

It can be seen, that our calculated bulk modulus value (59.19GPa) is in general in good agreement with the available theoretical data [3-6, 20, 21]; its deviation is only about 2.87% from the value calculated by the authors [1]LDA.

It is shown from figure 2, that the elastic constants  $C_{11}$ ,  $C_{12}$  and bulk modulus  $B$  increase monotonously when hydrostatic pressure is enhanced, whereas the elastic stiffness constants  $C_{44}$  increases very slowly with the elevated hydrostatic pressure to reach a its maximum value 40.3GPa at  $P= 4.5$ GPa; then decreased for the higher pressures to reach a value 37.95 GPa with  $P= 12$ GPa. We clearly observe a linear dependence in all curves of this compound (except for  $C_{44}$ , the variation is quadratic).



**Fig 2.** Elastic constants  $C_{ij}$  and the bulk modulus  $B$  versus the hydrostatic pressure of (B3) TIP

Our results for the pressure derivatives  $\partial C_{11}/\partial P$ ,  $\partial C_{12}/\partial P$ ,  $\partial C_{44}/\partial P$  and  $\partial B/\partial P$  at zero-pressure of (B3) TIP are listed in table 3, and compared with the available theoretical data [5]. It is easy to observe that the elastic constants  $C_{11}$ ,  $C_{12}$  and  $C_{44}$  as well as bulk modulus  $B$  exhibit linear increasing trends when pressure is enhanced. Further, the pressure derivative  $\partial C_{12}/\partial P$  is slightly smaller than  $\partial C_{11}/\partial P$ . It is easy to observe also that our results for the pressure derivatives  $\partial C_{11}/\partial P$ ,  $\partial C_{12}/\partial P$ ,  $\partial C_{44}/\partial P$  and  $\partial B/\partial P$  are relatively smaller than the results of Shi et al [5].

**Table 3.** Pressure derivatives of elastic constants  $\partial C_{ij}/\partial P$  and bulk modulus  $\partial B/\partial P$  at zero-pressure for (B3) TIP

Parameter	Our work	Other works
$\partial C_{11}/\partial P$	3.60	4.529 [5]GGA
$\partial C_{12}/\partial P$	3.91	4.833 [5]GGA
$\partial C_{44}/\partial P$	0.35	0.392 [5]GGA
$\partial B/\partial P$	3.81	4.732 [5] GGA

The mechanical properties as ductility and brittleness of semiconductor materials are of substantial importance and they can be obtained directly by using the elastic stiffness constants [22]. An empirical relationship has been mentioned by Pugh et al [23] between the plastic properties of polycrystalline pure metals and their elastic constants (bulk modulus  $B$  and shear modulus  $G$ ). Accordingly to the numerical value of the ratio  $R_{G/B}$ , we can deduce the nature of the studied material. If  $R_{G/B} < 0.5$ , the material behaves in a ductile manner, otherwise (i. e. if  $R_{G/B} > 0.5$ ) it behaves in a brittle manner [22]. The pressure dependency of the ratio  $R_{G/B}$  is illustrated in figure 3. For TIP compound, figure 3 shows that it is of ductile in nature from 0 to 12GPa.

Frantsevich [24] use another quantity (Poisson’s ratio  $\nu$ ) to distinguish the ductility and brittleness natures of the semiconductor material. According to Frantsevich rule, the critical value of  $\nu$  which separates ductile and brittle nature of material is 0.33. So, if the value of the  $\nu$  is less than 0.33, the material is considered brittle; otherwise (i. e. if  $\nu$  is more than 0.33) the material behaves in a ductile manner [22]. The pressure dependency of  $\nu$  according to Frantsevich rule is illustrated in figure 3. Accordingly, for TIP compound, figure 3 shows that it is of brittle in nature from 0 to 3.45GPa and is ductile nature with the increasing in pressure up to 12GPa.

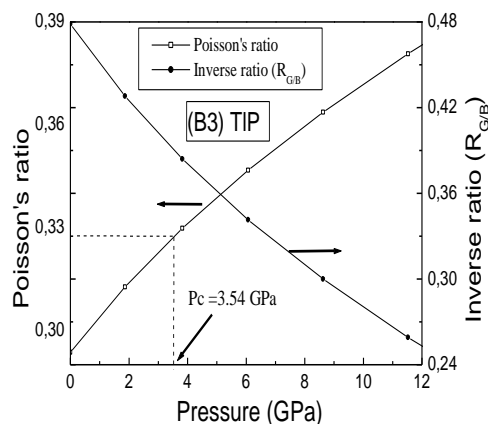


Fig 3. Variation of Poisson's ratio  $\nu$  and ratio  $R_{G/B}$  with pressure of (B3) TIP compound

The Poisson's ratio  $\nu$  in terms of the bulk modulus  $B$  and the Voigt averaged shear modulus  $G$  can be given as [22]

$$\nu = \frac{1}{2} \left( 3 \frac{B}{G} - 2 \right) \left( 3 \frac{B}{G} + 1 \right)^{-1} \quad (3)$$

According to Pugh [24], the ratio  $\Phi = B/G > 1.75$ , the material behaves in a ductile manner, otherwise the material behaves in a brittle manner. It follows that the empirical Pugh's critical value  $\Phi = B/G = 1.75$  which corresponds to inverse ratio:  $R_{G/B} = 0.571$  and also corresponds to  $\nu = 0.26$ , so that both Pugh et al [23] and Frantsevich et al [24] empirical rules only differ on the exact border between the two types of mechanical behavior [22]. According to Pugh's critical value, and from the Fig. 3, we can see that the TIP compound is of ductile in nature from 0 to 12GPa.

### 3.3. Mechanical Stability Criteria

To study the structural stability in (B3) TIP compound, the calculated values of the elastic constants at normal and under hydrostatic pressure were compared with the generalized elastic stability criteria using the following relations:

$$K = \frac{1}{3} (C_{11} + 2C_{12} + P) > 0, \quad G = \frac{1}{2} (C_{11} - C_{12} - 2P) > 0, \quad \text{and} \quad G' = (C_{44} - P) > 0 \quad (4)$$

As pressure is applied to (B3) TIP compound, it gets transformed from the zinblende phase into the site-ordered NaCl phase.

As shown in figure 4, we found that  $G$  decreases gradually with the pressure and vanishes at about 13.46 GPa, indicating that the ZB structure becomes mechanically unstable when pressure approaches the static phase transition value of 12.26 GPa, which supports the conclusion of transition to RS phase. This value (13.46 GPa) of the transition pressure obtained by us from the generalized stability criteria of Bohr is in good accordance with the value obtained from the application of the Enthalpies (12.26 GPa).

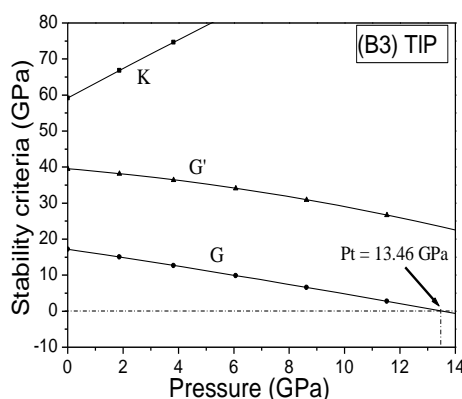


Fig 4. Generalized elastic stability criteria,  $G$ ,  $G'$  and  $K$  varying with the pressure of (B3) TIP

### 3.4. Direct and Converse Piezoelectric Coefficients

The piezoelectric tensor in the direct piezoelectric effect, contains only one constant ( $e_{14}$ ), is expressed  $C/m^2$ . In the converse piezoelectric effect, the piezoelectric tensor contains also only one constant  $d_{14}$  is expressed  $10^{-12}m/v$ , or in  $pC/N$ . These two piezoelectric tensors are given respectively as [25, 26]:

$$\underline{e} = \begin{pmatrix} 0 & 0 & 0 & e_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & e_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & e_{14} \end{pmatrix}, \quad \text{and} \quad \underline{d} = \begin{pmatrix} 0 & 0 & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{14} \end{pmatrix} \quad (5)$$

Calculations of the second-order elastic stiffness constant  $C_{44}$  and the direct piezoelectric coefficient ( $e_{14}$ ), we can determine the converse piezoelectric coefficients ( $d_{14}$ ) from the following formula [17]:

$$d_{14} = e_{14} / C_{44} \quad (6)$$

The effect of the hydrostatic pressure on the direct piezoelectric coefficient ( $e_{14}$ ) and the converse piezoelectric coefficient ( $d_{14}$ ) of (B3) TIP compound is presented in figure 5. As shown in this figure, both the direct and the converse piezoelectric coefficients increase gradually with the increasing of the hydrostatic pressure, where the one first takes the value of  $-0.1168 C/m^2$  at zero-pressure, and reaches the value  $0.435 C/m^2$  at  $P=12GPa$ , and the second one takes the value  $-3 \times 10^{-12} m/V$  at  $P=0$ , and reaches the value  $11.6 \times 10^{-12} m/V$  at pressure of 12 GPa.

In figure 5, the obtained values of both the direct and the converse piezoelectric coefficients for (B3) TIP compound are plotted against pressure  $p$ . The Analytical relations for the pressure dependence of (B3) thallium - phosphide of both  $e_{14}$  and  $d_{14}$  are given by the following a quadratic fit:

$$e_{14} = -0.1168 + 6.42 \times 10^{-2}p - 1.51 \times 10^{-3}p^2 \quad (7-a)$$

$$d_{14} = -2.85 + 1.51p - 2.53 \times 10^{-2}p^2 \quad (7-b)$$

Unfortunately, to our knowledge, no theoretical values and experimental data of  $e_{14}$  and  $d_{14}$  under high pressure are available for our comparison. Thus, further experimental investigations and theoretical predictions are significantly needed.

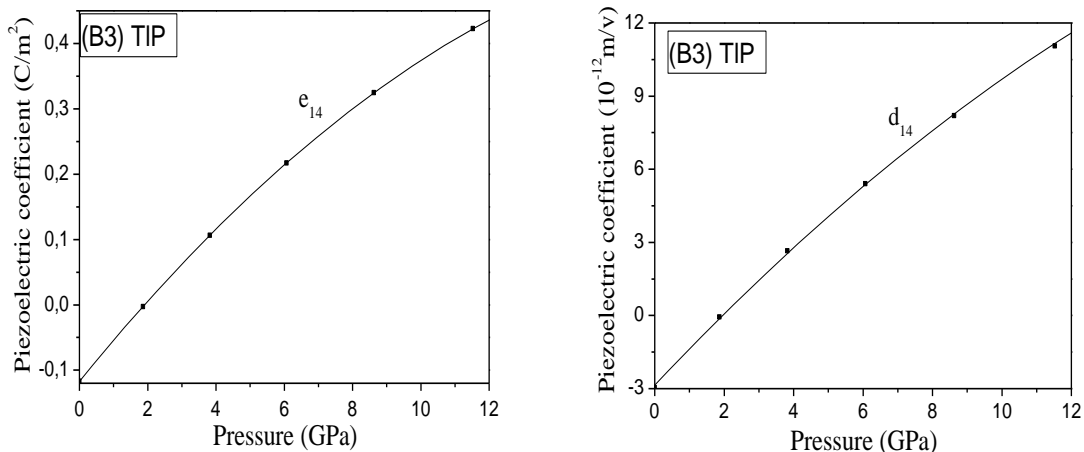


Fig 5. Hydrostatic pressure effect on direct and converse piezoelectric coefficients for (B3) TIP

### 3.5. Sound Velocity, Debye Temperature, Melting Temperature and Grüneisen Parameter

The sound velocities in anisotropic solid materials are strongly dependent on the directions of propagation. In general two types of waves are observed in crystalline solids: the longitudinal waves and the shear waves. At low temperature, the bulk sound velocity  $v$  depends on the crystal density  $g$  and the elastic constant  $C_{ij}$ . For the cubic zincblende crystals, the average acoustic velocity is given by the following formula [17, 26]:

$$v_m = \left[ \frac{1}{3} \left( \frac{2}{v_l^3} + \frac{1}{v_t^3} \right) \right]^{-1/3} \quad (8)$$

Where:  $v_l$  and  $v_t$  are respectively, the longitudinal and transverse elastic wave velocities. They are obtained by using of the isotropic shear modulus  $G$ , the bulk modulus  $B$  and the density  $g$  from Navier's equation [17]

$$v_l = \left( \frac{(3B + 4G)}{3g} \right)^{1/2}, \quad \text{and} \quad v_t = \left( \frac{G}{g} \right)^{1/2} \quad (9)$$

The isotropic shear modulus is given by:  $G = (G_V + G_R)/2$ ,

Where:  $G_V$  is the Voigt modulus, and  $G_R$  is the Reuss modulus, they are given by the following formulas:

$$G_V = \frac{(C_{11} - C_{12} + 3C_{44})}{5}, \quad \text{and} \quad G_R = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})} \quad (10)$$

The calculated values of the longitudinal ( $v_l$ ), transverse ( $v_t$ ) and average ( $v_m$ ) sound velocities of (B3) TIP at zero-pressure are presented in table 4 and compared with the available theoretical data [4-6]. It is seen that, our calculated values of the different types of sound velocities are in good accordance with data available in the literature [4-6].

It is worth noting, that the numerical value 2155.5 m/s of the average sound velocity ( $v_m$ ) obtained by Ciftci et al [4], seems to be inaccurate (wrong), because the later authors used the same formula as that used in this work (formula (8)), so the right value of  $v_m$  is 2275.07m/s. Hence, the result found by us for  $v_m$  is deviating from the value of the authors [4] only by the difference of 3.84%. It can also be seen, our calculated transverse sound velocity is very good agreement with the values of the other calculations [4, 5], it deviates with 4.35% from the value calculated by Ciftci et al [4].

One of the standard methods to calculate the Debye temperature ( $\theta_D$ ) is from elastic constants data; it may be estimated from the average sound velocity  $v_m$  with the means of the following equation [27]

$$\theta_D = \frac{h}{k_B} \left( \frac{3q}{4\pi} \frac{Ng}{M} \right)^{1/3} v_m \quad (11)$$

Where:  $h$  is the Planck constant;  $k_B$  is the Boltzmann constant (so the report (ratio):  $h/k$  have the usual meanings of quantum mechanics),  $N$  is Avogadro's number,  $g$  is the density,  $M$  is the molecular weight and  $q$  is the number of atoms in the molecule (in our case  $q = 2$  for (B3) TIP).

If we make the appropriate simplifications for the zinc-blende (B3) phase, the Debye temperature may be estimated from the average sound velocity  $v_m$  (in km/s) and lattice parameter  $a$  (in Å) by means of the following equation:

$$\theta_D \approx 595.467 \frac{v_m}{a} \quad (12)$$

The calculated Debye temperature  $\theta_D$  of (B3) TIP at zero-pressure is about 218.47K. It is listed in table 4, and compared with the available theoretical data [4-6].

The melting point of a substance is considerably affected by the pressure and usually depends on temperature. The melting temperature of several cubic crystalline solid can be estimated by the following empirical relation [28]

$$T_m = 553 + (591/Mbar) C_{11} \pm 300K \quad (13)$$

The calculated melting point  $T_m$  of (B3) TIP at zero-pressure is about 1038.51±300K. It is listed in table 4, and compared with the available theoretical data [4, 5].

Recently, Kumar et al. [29] proposed a linear relation between the Debye temperature ( $\theta_D$ ) and the melting temperature ( $T_m$ ), it is given by the following empirical formula:

$$\theta_D = -K_1 + K_2 (T_m) \tag{14}$$

The values of the constants  $K_1$  and  $K_2$  are respectively: 153.40 and 0.354 for  $A^{III}B^V$  semiconductors. Using eq. (14) and the value (1038.51K) of the melting temperature, the value of  $\theta_D$  have been calculated, is about 214.23K; it's listed in table 4 and compared with the available theoretical data [4-6].

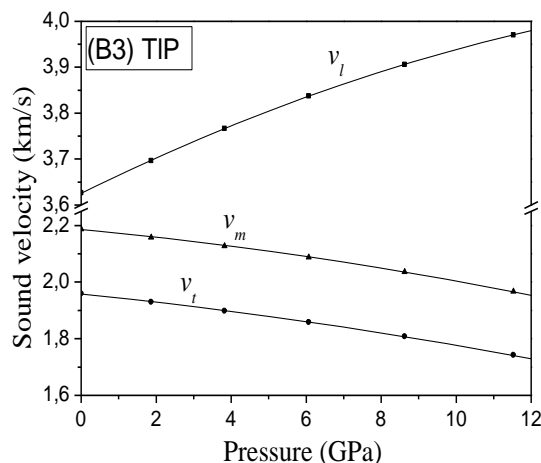
It is worth noting also, that the value 302K of the Debye temperature obtained in previous work [4], seems to be also inaccurate, because the later authors used the same formula as that used in this work (formula (12)), so the right value of  $\theta_D$  is 235.73K. Hence, the result (218.47K) found in the present work for  $\theta_D$  is deviating from the value of Ciftci et al [4] by the difference of 7.32%.

**Table 4.** Longitudinal ( $v_l$ ), transverse ( $v_t$ ), and average ( $v_m$ ) sound velocities, Debye temperature  $\theta_D$  and melting temperature  $T_m$  of (B3) TIP at zero-pressure in comparison with available theoretical values [4-6]. <sup>a</sup> from the relation of Eq. (12), <sup>b</sup> from the relation of Eq. (14)

Parameter	Our work		Other works	
$v_l$ (m/s)	3626.36		3547.3 [4]	3521.5[5] 4760[6]
$v_t$ (m/s)	1960.10		2049.4 [4]	1983.2[5] 2858[6]
$v_m$ (m/s)	2187.63		2275.07 [4] (Right value)	2583.4[5] 3161[6]
$\theta_D$ (K)	218.47 <sup>a</sup>	214.23 <sup>b</sup>	235.73 [4] (Right value)	256.4[5] 346[6]
$T_m$ (K)	1038.51±300		1112±300[4] (Right value)	999±300[5]

The value 1697±300K of melting temperature obtained in previous work [4], seems to be also inaccurate, because the later authors used the value ( $C_{11}=94.63\text{GPa}$  so  $0.9463\text{Mbar}$ ) to estimate the value of  $T_m$ , and if we use this value ( $C_{11}=0.9463\text{Mbar}$ ) in the formula (14), we obtain the result ( $T_m = 1112.26\pm 300\text{K}$ ). Hence, the result found in the present work for the melting temperature is deviating from the value of the authors [4] only by the difference of 6.63%.

The dependence of longitudinal ( $v_l$ ), transverse ( $v_t$ ) and average ( $v_m$ ) sound velocities versus the hydrostatic pressure of the TIP are plotted in figure 6.



**Fig 6.** Sound velocities versus the pressure of (B3) TIP compound

It is shown in figure 6 that the longitudinal sound velocity ( $v_l$ ) increases monotonously when pressure is enhanced, on the other hand, the transverse ( $v_t$ ) and average ( $v_m$ ) sound velocities decrease slowly with the elevated pressure.

In figure 6, the obtained values of the longitudinal ( $v_l$ ), the transverse ( $v_t$ ) and average ( $v_m$ ) sound velocities for (B3) TIP compound are plotted against pressure  $p$ . Three Analytical relations for the pressure dependence of (B3) thallium - phosphide longitudinal ( $v_l$ ), transverse ( $v_t$ ) and average ( $v_m$ ) sound velocities are given by the following a quadratic fit:

$$v_l = 3.626 + 4.018 \times 10^{-2} p - 8.889 \times 10^{-4} p^2 \tag{15-a}$$



$$v_m = 2.186 - 1.237 \times 10^{-2} p - 5.821 \times 10^{-4} p^2 \quad (15-b)$$

$$v_t = 1.958 - 1.355 \times 10^{-2} p - 4.600 \times 10^{-4} p^2 \quad (15-c)$$

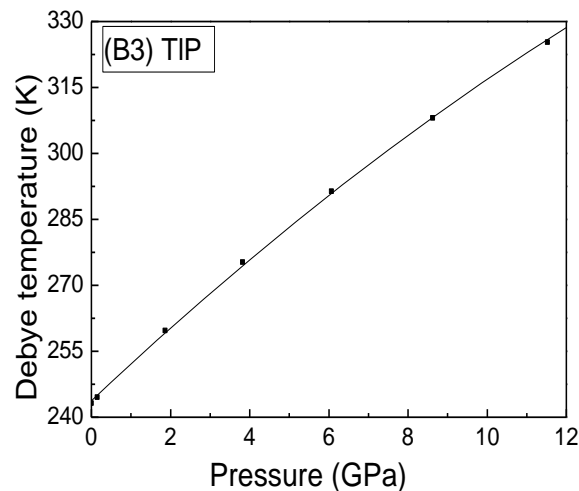
The dependence of the sound velocities of (B3) TIP compound is studied in the previous work of Singh and Sarwan [6] by means of the Interaction Potential Model (IPM). It is shown in a figure 7(b) in the work of Singh and Sarwan [6], that the longitudinal sound velocity increases monotonously when pressure is enhanced, like this obtained in our work, but contrary to our results, the transverse ( $v_t$ ) and average ( $v_m$ ) sound velocities increase with the increasing of hydrostatic pressure.

The Grüneisen parameter  $\zeta$  is an important parameter in solid state matter because is relate to lattice vibration phenomena [30]. This parameter is dependents of longitudinal ( $v_l$ ) and transverse ( $v_t$ ) sound velocities, which is evaluated using the following expression [30]:

$$\zeta = \frac{9(v_l^2 - (4/3)v_t^2)}{2(v_l^2 + 2v_t^2)} \quad (16)$$

Using Eq. (16), the numerical value of the Grüneisen parameter for (B3) TIP at equilibrium lattice parameter have been calculated and found to be 1.734. Unfortunately as far as we know, there is no data available in the literature on the Grüneisen parameter for (B3) TIP compound. Thus, further experimental investigations and theoretical predictions are significantly needed.

In order to obtain the pressure influence on the Debye temperature  $\theta_D$ , the quasi-harmonic Debye model [31] is applied. The value obtained of  $\theta_D$  at zero-pressure is about 243.76K. It can be seen, that our calculated value of Debye temperature  $\theta_D$  (243.76 K) is in very good agreement with the value obtained by Shi et al [5]; the deviation between the two values is only about 4.93%. The results of Debye temperature  $\theta_D$  obtained at different values of pressure are plotted in figure 7.



**Fig 7.** Debye temperature  $\theta_D$  versus the pressure of (B3) TIP compound

The Analytical relation for the pressure dependence of (B3) thallium - phosphide of the Debye temperature  $\theta_D$  is given by the following a quadratic fit:

$$\theta_D = 243.76 + 8.48 p - 11.71 \times 10^{-2} p^2 \quad (17)$$

It is noted that the Debye temperature of (B3) TIP compound tend to increases with increasing hydrostatic pressure to reach a value 328.42 K at pressure of 12 GPa.

#### 4. CONCLUSION

The density functional perturbation theory (DFPT) and the density functional theory (DFT) methods have been used to obtain the independent elastic constants, the bulk modulus, the longitudinal, transverse, and average sound velocity and the Debye temperature at zero-pressure and under hydrostatic pressure of (B3) TIP compound. In general at zero-pressure, the majority of

these quantities obtained by us are relatively lower than the values obtained by the previous theoretical data reported in the literature.

The melting temperature and the Grüneisen parameter at equilibrium lattice parameter are also obtained. Our value of the melting temperature is in good agreement with other theoretical results.

By mean of the Poisson's ratio  $\nu$  and the ratio  $R_{G/B}$ , we estimate the critical value of pressure which separates ductile and brittle nature.

The effects of the hydrostatic pressure on the direct and the converse piezoelectric coefficients, on the sound velocities and the Debye temperature of (B3) TIP compound are presented. All these parameters increase gradually with the increasing of the hydrostatic pressure. Except, the transverse and average sound velocities decrease slowly with the elevated pressure.

The pressure phase transition from the zincblende phase to Rock-salt phase of this compound is obtained with two different methods; it is at around 12.26 GPa and 13.46 GPa respectively. All our values obtained respectively from the enthalpy and the generalized elastic stability criteria are much higher than the other theoretical data.

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