1. Introduction

The rare earth (RE) yttrium compounds: YS, YSe and YTe belong to the class of yttrium mono-chalcogenides that crystallize in the NaCl structure (B1) and discerns superconductivity with transition temperature in the range of 1.3–2.5 K [1]. Gschneidner and co-workers [2,3] have reported the elaboration of yttrium chalcogenides by a direct combination of the pure rare earth metal and pure chalcogen element. Mohite and Lokhande [4] have reported the electro synthesis of yttrium chalcogenides by a direct combination of the pure rare earth metal and pure chalcogen element. Mohite and Lokhande [4] have reported the synthesis of yttrium chalcogenides using both X-ray diffraction experiments and the full potential linear muffin–tin orbital method. They have found that YS, YSe and YTe crystallize in NaCl structure at ambient conditions and undergo a structural phase transition at 53.0, 36.0 and 14.0 GPa, respectively [6].

In a previous work [5], we have noticed that under compression, the YS, YSe and YTe compounds undergo a structural phase transition from the NaCl (B1) phase to the CsCl (B2) phase at 49.45, 28.44 and 11.22 GPa, respectively. Very recently, Vaitheeswaran and co-authors [6] have studied the high pressure structural phase transitions of yttrium chalcogenides using both X-ray diffraction experiments and the full potential linear muffin–tin orbital method. They have found that YS, YSe and YTe crystallize in NaCl structure at ambient conditions and undergo a structural phase transition to the CsCl structure at 53.0, 36.0 and 14.0 GPa, respectively [6].
knowledge this is the first quantitative theoretical predictions on YX monochalcogens and still awaits experimental confirmation.

The elastic constants determine the response of a crystal to the external forces, and obviously play an important role in determining the strength of materials with respect to the changes in the external macroscopic variables, such as pressure and temperature effects. Furthermore, the knowledge of these constants is essential to interpret the thermodynamic and thermoelastic properties of solids. Therefore, the study of temperature dependence of the elastic moduli is of substantial importance enabling us to provide detailed understanding of the thermoelastic behavior of solids at high temperatures, which is the second objective of the present work. To address this interest, in this work, we investigate the structural, thermodynamic and elastic properties at high pressures and temperatures, by using first-principles calculations combined with the quasi-harmonic Debye model.

This paper is organized as follows: In Section 2, we briefly describe the computational techniques used in this work. Results and discussions of the structural, thermodynamic and elastic properties are presented in Section 3. Finally, conclusions and remarks are given in Section 4.

2. Computational method

The zero temperature energy calculations are performed using FP-LAPW method implemented in Wien2k computer package [7]. The space in this method is divided into an interstitial region (IR) and non overlapping muffin-tin (MT) spheres centered at the atomic sites. Exchange and correlation functional is given by the generalized-gradient approximation of Perdew et al. (GGA96) [8]. The valence wave functions inside the muffin–tin spheres are expanded up to $l_{\text{max}} = 10$. The wave functions in the interstitial regions are expanded in terms of plane waves (PWs). The wave functions and derivatives are made continuous at the boundary of the spheres, and there is no shape approximations imposed on either the crystalline charge density or potential. The PWs cut-off was used with the highly recommended condition $R_{\text{MT}}K_{\text{max}} = 9$, where $R_{\text{MT}}$ is the average of the muffin–tin spheres, and the $K_{\text{max}}$ is the PW cut-off. The sphere radii used in the calculations for both B1 and B2 structure are 2.5, 2.2, 2.32 and 2.5 a.u. for Y, S, Se and Te, respectively. The k-integration over the Brillouin zone was performed using a mesh of 56 k-points in the irreducible wedge of the Brillouin zone. To ensure proper convergence of the self-consistency calculation, the calculated total energy of the crystal converged to less than 0.1 mRy.

Usually, the first-principles calculations have been done for $T = 0$ K, where there is no thermal excitation of nuclei. Attempts were made to allow for the contribution of the thermal excitation of nuclei to thermodynamic functions without using empirical parameters. There are two directions followed in those attempts. The first uses the Debye model; the second is based on the approximate construction of the phonon dispersion relations. The new feature, which allows describing the results as first-principles, is the use of values obtained in first-principles calculations instead of empirical parameters [9]. Based on the phonon properties, which can be successfully predicted by the first-principles density functional theory, one can obtain the free energy within quasi-harmonic approximation, and then the thermodynamic properties. Unfortunately this method is not yet implemented in Wien2K. In our present study the investigation of thermal effects were done within the quasi-harmonic Debye theory of crystals. From an energy–volume ($E–V$) relationship in the static approximations, obtained via first-principles calculations, the quasi-harmonic Debye model [10–14], implemented in Gibbs program [10], allows us to calculate all thermodynamic parameters that depend on temperature and pressure which are used to derive other macroscopic properties. In this model, the non-equilibrium Gibbs function $G^*(V, P, T)$ has the following form:

$$G^*(V, P, T) = E(V) + PV + A_{\text{ vib}}(\Theta_D(V), T)$$

(1)

here $E(V)$ is the total energy as a function of the unit cell volume, $V$ is the hydrostatic pressure, $\Theta_D(V)$ is the Debye temperature as a function of $V$, and $A_{\text{ vib}}$ is the vibrational Helmholtz free energy (see Ref. [10] for more details) which can be expressed as [10]:

$$A_{\text{ vib}}(\Theta_D; T) = nk_BT \left[ \frac{9}{8} \Theta_D^3 + 3 \ln(1 - e^{-\Theta_D/T}) - D(\Theta_D/T) \right]$$

(2)

here $n$ is the number of atoms per formula unit, $k_B$ is the Boltzmann constant and $D(\Theta_D/T)$ represents the Debye integral. The Debye characteristic temperature of the solid, $\Theta_D$ in Eq. (1), is related to an average sound velocity, since in Debye’s theory the vibrations of the solid are considered as elastic waves. Assuming an isotropic solid, with Poisson’s ratio $\sigma$, $\Theta_D$ can be calculated as:

$$\Theta_D = \frac{h}{k_B} \left[ \frac{9}{8} \Theta_D^3 + 3 \ln(1 - e^{-\Theta_D/T}) - D(\Theta_D/T) \right]$$

(3)

where $M$ is the molecular mass per unit cell, $B_S$ is the adiabatic bulk modulus, which can be approximated by the static compressibility:

$$B_S = \frac{dV}{dP} \left( \frac{E(V)}{V} \right)$$

(4)

and $f(\sigma)$ is given by:

$$f(\sigma) = \left\{ 3 \left[ 2 \left( \frac{21 + 8 K}{31 - 2 \sigma} \right)^{3/2} + \left( \frac{11 + \sigma}{31 - \sigma} \right)^{3/2} \right]^{-1/3} \right\}$$

(5)

Therefore, the non-equilibrium Gibbs functions $G^*(V, P, T)$ as a function of $(V, P, T)$ can be minimized with respect to volume $V$:

$$\frac{dG^*(V, P, T)}{dV} \bigg|_{P,T} = 0$$

(6)

By solving Eq. (6), one can get the thermal equation of state (EOS) $V(P, T)$. The isothermal bulk modulus $B_T$, the heat capacity at constant volume $C_V$, the heat capacity at constant pressure $C_P$ and the thermal expansion coefficient $\alpha$ are given by:

$$B_T(P, T) = V \left( \frac{d^2G^*(V, P, T)}{dV^2} \right) \bigg|_{P,T}$$

(7)

$$C_V = 3nk_BT \frac{dE(V)}{dV} \bigg|_{P,T} - \frac{3E_0}{e^{\Theta_D/T} - 1}$$

(8)

$$C_P = C_V (1 + \alpha T)$$

(9)

$$\alpha = \frac{V}{C_P} \frac{dV}{dP}$$

(10)

where $\gamma$ is the Gr"uneisen parameter, which is given by:

$$\gamma = -\frac{\alpha}{\lambda} \frac{d\lambda}{dV}$$

(11)

3. Results and discussions

3.1. Static structural and elastic properties

Initially, the calculated total energies ($E_{\text{tot}}$) of both B1 and B2 phases of the herein studied materials for different volumes ($V$) of the unit cell at zero pressure and temperature are fitted to the Murnaghan equation of state (EOS) [15]. From the least square fitting of the ($E_{\text{tot}} - V$) data to the Murnaghan EOS, we obtain the
equilibrium volume $V_0$, bulk modulus $B_0$ and pressure derivative of the bulk modulus $B'$ for both phases of the yttrium RE compounds (RE = S, Se, Te). The obtained results are summarized in Table 1 along the existing experimental and theoretical data in the sake of comparison. It is interesting to comment that with increased chalcogen size, the lattice get expanded in both B1 and B2 phases. Also at zero pressure and at zero temperature the lattice of yttrium RE compounds gets softened with increased chalcogen size. Our obtained results are in good agreement with the existing experimental findings [16–20]. The deviations of the calculated optimized lattice constant ($a_0$) values from the measured data are less than 1% for all herein studied compounds. This may be an indication of the capability of this chosen first-principles method to product reliable and accurate results.

The elastic properties of a cubic crystal are described by three independent elastic constants: $C_{11}$, $C_{12}$ and $C_{44}$. Ab initio calculation of the elastic constants requires precise methods. For obtaining the elastic constants of the YS, YSe and YTe compounds in both B1 and B2 phases, a popular approach [21–23], which is based on the analysis of the changes in calculated total energy values resulting from changes in the strain, is used. Table 2 lists our results for the elastic constants $C_{ij}$ at zero pressure and zero temperature compared with the existing data in the literature [6,24,25]. There are available experimental data only for YS in B1 phase [25]. Taking into account the difficulties to grow single-crystals and to measure the $C_{ij}$ values, our theoretical values agree with the existing measured values for the YS B1 phase within the experimental errors. Our computed values for $C_{11}$ and $C_{12}$ are in excellent agreement with the measured ones: their differences are 4–7%. Our calculations overestimate the $C_{44}$ value by 25% compared to the measured one [25]. There are no available results for the elastic constants $C_{ij}$ of the herein studied materials in B2 phase. All these constants are positive and satisfy the generalized criteria for mechanically stable crystals [26]: $C_{11} - C_{12} > 0$; $C_{11} + 2C_{12} > 0$; $C_{44} > 0$. It is informative to mention that with increased chalcogen size second order elastic constants $C_{ij}$ suffers decreasing trend leading to the softening of yttrium RE lattice.

We note here that the reported $C_{ij}$ are estimated using first-principles calculations for single-crystals. However, large single-crystals are currently unavailable and consequently measurements of the individual elastic constants are impossible. The bulk modulus $B$ and shear modulus $G$ may be determined experimentally on the polycrystalline samples to characterize their mechanical properties. Theoretically, the calculated elastic constants of a single-crystal allows us to obtain its macroscopic mechanical properties of its bulk polycrystalline form, namely bulk modulus $B$ and shear modulus $G$, via the Voigt–Reuss–Hill approximations [27–29]. Here, Voigt and Reuss approximations represent extreme values, and Hill recommended that the arithmetic mean of these two

### Table 1

<table>
<thead>
<tr>
<th>Phase</th>
<th>$a_0$ (Å)</th>
<th>$B_0$ (GPa)</th>
<th>$B'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>YS-B1</td>
<td>Present: 5.523 (5.536)</td>
<td>98.8 (97.5)</td>
<td>4.28 (4.26)</td>
</tr>
<tr>
<td></td>
<td>Expt.</td>
<td>5.492$^a$, 5.489$^a$, 5.495$^a$, 5.50$^b$, 5.466$^b$</td>
<td>96.9$^a$, 93$^b$</td>
</tr>
<tr>
<td>YS-B2</td>
<td>Present: 3.417 (3.426)</td>
<td>89.3 (87.6)</td>
<td>4.2 (4.4)</td>
</tr>
<tr>
<td>YSe-B1</td>
<td>Present: 5.759 (5.775)</td>
<td>82.7 (81.5)</td>
<td>4.3 (4.2)</td>
</tr>
<tr>
<td></td>
<td>Expt.</td>
<td>5.711$^c$, 5.701$^c$, 5.703$^c$</td>
<td>82$^b$</td>
</tr>
<tr>
<td></td>
<td>Others [6]</td>
<td>5.736</td>
<td>85.5</td>
</tr>
<tr>
<td>YSe-B2</td>
<td>Present: 3.560 (3.571)</td>
<td>76.5 (75.7)</td>
<td>4.1 (3.9)</td>
</tr>
<tr>
<td>YTe-B1</td>
<td>Present: 6.152 (6.171)</td>
<td>65.5 (64.5)</td>
<td>4.2 (4.1)</td>
</tr>
<tr>
<td></td>
<td>Expt.</td>
<td>6.093$^a$, 6.103$^a$, 6.095$^a$</td>
<td>67$^b$</td>
</tr>
<tr>
<td>YTe-B2</td>
<td>Present: 3.771 (3.783)</td>
<td>68.6 (66.8)</td>
<td>4.3 (4.4)</td>
</tr>
</tbody>
</table>

$^a$ Ref. [1].
$^b$ Ref. [6].
$^c$ Ref. [16].
$^d$ Ref. [17].
$^e$ Ref. [18].
$^f$ Ref. [19].
$^g$ Ref. [20].

### Table 2

<table>
<thead>
<tr>
<th>Phase</th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{44}$</th>
<th>$B$</th>
<th>$G_V$</th>
<th>$G_R$</th>
<th>$G_H$</th>
<th>$E$</th>
<th>$T_m \pm 300$ K</th>
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<tbody>
<tr>
<td>YS</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fm$ar{3}$m</td>
<td>Present: 237.5</td>
<td>27.9</td>
<td>22.3</td>
<td>97.8</td>
<td>32.5</td>
<td>55.3</td>
<td>43.9</td>
<td>114.6</td>
<td>1956</td>
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<tr>
<td></td>
<td>Expt.</td>
<td>250$^a$</td>
<td>20$^a$</td>
<td>30$^a$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2060$^{b}$</td>
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<td></td>
<td>Other [6]</td>
<td>284.7</td>
<td>12.1</td>
<td>21.6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pm$ar{3}$m</td>
<td>Present: 193</td>
<td>35.4</td>
<td>36.1</td>
<td>88.2</td>
<td>46.09</td>
<td>53.18</td>
<td>49.6</td>
<td>125.4</td>
<td>1693</td>
</tr>
<tr>
<td>YSe</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fm$ar{3}$m</td>
<td>Present: 201.2</td>
<td>22.7</td>
<td>8.6</td>
<td>82.2</td>
<td>13.4</td>
<td>40.8</td>
<td>27.1</td>
<td>73.4</td>
<td>1742</td>
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<tr>
<td></td>
<td>Other [6]</td>
<td>239.1</td>
<td>9.6</td>
<td>11.2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pm$ar{3}$m</td>
<td>Present: 154.1</td>
<td>37.1</td>
<td>28.4</td>
<td>76.1</td>
<td>35.76</td>
<td>40.44</td>
<td>38.1</td>
<td>97.9</td>
<td>1463</td>
</tr>
<tr>
<td>YTe</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fm$ar{3}$m</td>
<td>Present: 160.5</td>
<td>17</td>
<td>7.8</td>
<td>64.8</td>
<td>12.2</td>
<td>33.4</td>
<td>22.8</td>
<td>61.2</td>
<td>1501</td>
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<tr>
<td></td>
<td>Other [6]</td>
<td>198.9</td>
<td>2</td>
<td>4.2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pm$ar{3}$m</td>
<td>Present: 138.4</td>
<td>32.2</td>
<td>26.1</td>
<td>67.6</td>
<td>31.1</td>
<td>34.7</td>
<td>32.9</td>
<td>89.3</td>
<td>1370</td>
</tr>
</tbody>
</table>

$^a$ Ref. [25].
$^b$ Ref. [26].
limits is used as effective moduli in practice for polycrystalline samples. Their definitions for cubic systems are as follows [30]:

\[
B_V = B_R = B_{H} = \frac{(C_{11} + 2C_{12})}{3}
\]

(12)

\[
G_V = \frac{(C_{11} - C_{12} + 3C_{44})}{5}
\]

(13)

\[
G_R = 5\frac{(C_{11} - C_{12})C_{44}}{[4C_{44} + 3(C_{11} - C_{12})]}
\]

(14)

In this way, when a bulk modulus \( B_R \) and a shear modulus \( G_H \) are obtained from Eqs. (12) and (13), one can calculate the averaged Young’s modulus \( E \) by the expression

\[
E = 9B_H/[1 + (3B_H/G_H)]
\]

(15)

Table 2 illustrates the calculated values of the elastic parameters for the polycrystalline Y(S, Se, Te) species. The bulk moduli of these three considered materials are quite small; since a strong correlation exists between the bulk modulus and hardness of materials, so these materials should be classified as relatively soft materials with high compressibility. Pugh’s \( B/G \) ratio empirical criterion [31] is one of the widely used to provide information about brittle (ductile) nature of materials. If \( B/G > 1.75 \), a ductile behavior is predicted; otherwise, the material behaves in a brittle manner. According to the calculation results shown in Table 2, the \( B/G \) ratios of the studied compounds are higher than 1.75, i.e., indicating a ductile nature of these materials and thus they will be resistant to thermal shocks; their mechanic properties decrease slowly with increasing temperature.

Practically, all known crystals are elastically anisotropic, and a proper description of such anisotropic behavior has an important implication in engineering science as well as in crystal physics since the elastic anisotropy could introduce microcracks in materials [32,33]. Moreover, recent research demonstrates that the elastic anisotropy of crystals has a significant influence on the nanoscale precursor textures in alloys [34,35]. Therefore, several criteria have been developed to investigate the elastic anisotropy.

Although the herein considered compounds are cubic, they possess anisotropic elastic properties, which can be analyzed in three ways. First, the degree of anisotropy can be evaluated from the values of the upper (Voigt, \( G_V \)) and lower (Reuss, \( G_R \)) shear moduli by introducing the so-called anisotropy factor \( A_C \) [36]:

\[
A_C = (G_V - G_R)/(G_V + G_R).
\]

A value of zero represents elastic isotropy and a value of 1 (100%) is the largest possible anisotropy. Numerical calculation with the given values of \( G_V \) and \( G_R \) in Table 2 yielded: \( A_N^{\text{YS}} = 0.26 \), \( A_N^{\text{YTe}} = 0.51 \), \( A_N^{\text{YSe}} = 0.46 \), \( A_C^{\text{YS}} = 0.07 \), \( A_C^{\text{YTe}} = 0.06 \) and \( A_C^{\text{YSe}} = 0.05 \). These values indicate that these compounds are characterized by a strong elastic anisotropy and the B2 phase of these materials is less anisotropic than the B1 phase. The above elastic anisotropy criteria quantify the anisotropy degree from shear contribution. In order to quantify the extent of the anisotropy accurately, a new and more universal index \( A^W \) has been proposed by Ranganathan and Ostoj-Starzewski [37] to measure the single-crystal anisotropy accounting for both bulk and shear contributions, where the \( A^W \) is defined as follows:

\[
A^W = 5G_V/G_R + B_V/B_R - 6.
\]

For isotropic crystals, the universal index is equal to zero (\( A^W = 0 \)); the deviations of \( A^W \) from zero define the extent of crystal anisotropy. The values of the Young’s modulus in some different directions listed in Table 3 reveal that the studied materials are characterized by a strong anisotropy and the B1 phase is more anisotropic than the B2 phase.

The third way of treating elastic anisotropy is to plot a three-dimensional dependence of the Young’s modulus \( E \) on given direction in a crystal. Three-dimensional (3D) surface representation of the elastic moduli is an effective method to visualize the elastic anisotropy of a material along its crystallographic directions. In 3D representation, an isotropic system would exhibit a spherical shape, and a deviation from spherical shape indicates the degree of anisotropy. So, for a deep look into the peculiar features of the elastic anisotropy of our herein studied materials we have plotted in Fig. 1 their direction-dependent Young’s modulus surface using the following relation [38]:

\[
E = \frac{1}{[S_{11} + 2(S_{11} - S_{12} - 1/(2S_{44})(n_1^2n_2^2 + n_2^2n_3^2 + n_3^2n_1^2)]}
\]

(15)

where \( S_{ij} \) are the elastic compliance constant that can be obtained through an inversion of the elastic constant matrix, and \( n_1, n_2 \) and \( n_3 \) are the directional cosines with respect to the \( x-, y- \) and \( z- \) axes, respectively. The shape of the surfaces plotted in Fig. 1 is far from spherical and exhibits a strong anisotropy. We have plotted also in Fig. 2 the cross-section of these surfaces in the \( (0 0 1), (1 0 0) \) and \( (1 1 0) \) coordinate planes. In the three considered compounds the highest value of the Young’s modulus \( E_{\text{max}} \) is realized for the external stress applied along the crystallographic axes \( a, b \) and \( c \) \( ([1 0 0], [0 1 0] \) and \( [0 1 0] \) directions), and the lowest value \( E_{\text{min}} \) is for the stress along the \( [1 1 1] \) direction. The lowest values, \( E_{\text{min}} \), and highest values, \( E_{\text{max}} \), of the Young’s modulus for the herein considered materials are given in Table 3. The estimated values of the \( E_{\text{min}}/E_{\text{max}} \) ratios indicate the strong elastic anisotropic behavior of these materials and the B2 phase is less anisotropic than the B1 phase.

Fine et al. [39] showed that there is a rough correlation between elastic constants and the melting temperature. For cubic metals this relation is given by: \( T_m = [553 K + (5.91 K/GPa)C_1] \pm 300 K \). The estimated values of the melting temperature for the herein considered materials are reported in Table 2 along with existing experimental findings. A good agreement between our calculated melting temperature of YS in B1 phase and the measured one [25] has been obtained. It is noticed that \( T_m \) decreases with increased chalcogen size or in other words the resistance to deformation by a stress suppresses. A reduced \( T_m \) infers the mechanical softening of the rare earth chalcogen lattice. Based on all above results, we conclude that the herein used ab-initio method accurately reproduced the experimental structural and elastic properties of the herein studied compounds. Therefore, we are confident that this approach can be used to study the temperature dependence of the elastic constants of these materials.

### 3.2. Temperature dependence of the structural, thermodynamic and elastic properties

From the calculated \( E-V \) data at \( T=0 K \) and \( P=0 \) GPa, and through the quasi-harmonic Debye, we have calculated the pressure and temperature dependencies of the structural and thermodynamic quantities of the YX \( (X=S, Se, Te) \) compounds in B1 and B2 phases. According to our results, YTe in B2 phase starts melting...

<table>
<thead>
<tr>
<th>System</th>
<th>( E ([1 0 0]) )</th>
<th>( E ([1 1 0]) )</th>
<th>( E ([1 1 1]) )</th>
<th>( E_{\text{min}}/E_{\text{max}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>YS</td>
<td>231.63</td>
<td>76.09</td>
<td>62.17</td>
<td>0.27</td>
</tr>
<tr>
<td>YTe</td>
<td>28.63</td>
<td>22.50</td>
<td>0.14</td>
<td></td>
</tr>
<tr>
<td>YSe</td>
<td>196.60</td>
<td>31.89</td>
<td>24.93</td>
<td>0.13</td>
</tr>
</tbody>
</table>

### Table 3
Calculated values of the Young’s modulus \( E \), in GPa, in the \([1 0 0], [1 1 0] \) and \([1 1 1] \) directions. \( E_{\text{min}} \) and \( E_{\text{max}} \) are the lowest value and highest values, respectively, of the Young’s modulus.
at 1370 K, so we have calculated the thermodynamics quantities at temperature ranging from 0 to 1200 K, where the quasi-harmonic model remains fully valid.

The obtained temperature dependence of the volume at zero pressure for all herein studied compounds is illustrated in Fig. 3(a). The volume is almost constant for temperatures less than 100 K and it increases remarkably with temperature for $T > 100$ K. Under compression, the calculation shows that YS, YSe and YTe undergo a structural phase transition from NaCl (B1) structure to CsCl (B2) structure. The calculated transition pressures are 49.45, 28.44 and 11.22 GPa for YS, YSe and YTe, respectively. The variation of volume versus pressure for the YS, YSe and YTe compounds in both B1 and B2 structures is plotted in Fig. 3(b). The volume increases with the increasing temperature and decreases with the increasing pressure. We have reported in Fig. 3(b) the results obtained experimentally and theoretically by Vaitheeswaran et al. [6] for the sake of comparison. There is a good agreement between our results and the theoretical data of Vaitheeswaran et al. [6].

There is also a reasonable agreement between our results and the existing experimental measurements [6] for the low pressures. Values of the lattice constant $a_0$ at zero pressure and 300 K for all herein studied materials are summarized in Table 1.

The obtained temperature dependence of the isothermal ($B_T$) and adiabatic ($B_S$) bulk moduli of the YS, YSe and YTe compounds in both B1 and B2 structures are depicted in Fig. 4. It can be seen that when $T < 100$ K, both $B_T$ and $B_S$ remains nearly constant; when $T > 100$ K, they drop remarkably with temperature $T$, which are in accordance with the fact that $V$ is almost constant at low temperature and increases with the increasing temperature as shown in Fig. 3(a). As temperature increases, the atoms go away from each other, and the interactions between these atoms become weaker and consequently the average atomic bond strength decreases, which explain the decrease of the bulk modulus. Temperature dependence curves of the $B_T$ and $B_S$ coincide at low temperature and then diverge with increasing temperature. At a given pressure and temperature, the values of

![Fig. 1. Directional dependence of the Young's modulus E for the YS, YSe and YTe materials in both B1 and B2 phases.](image-url)
isothermal and adiabatic bulk moduli of the B2 structure are smaller than that of B1 structure, except for YTe where the values of $B_T$ and $B_S$ for B1 are smaller than that of B2 up $T$ equal to 700 for $B_T$ and 800 K for $B_S$. It suggests that the B2 structure is more compressible than the B1 structure for the YS and YSe compounds; the exception is for YTe for temperature lower than 700 K.

The thermal expansion coefficient $\alpha$ reflects the temperature dependence of volume at constant pressure: $\alpha = \frac{1}{V} \frac{\partial V}{\partial T}/C_0/C_1 P$. The thermal expansion coefficient $\alpha$ is due to an anharmonic term in the cohesive energy for the small displacements of the atoms from their equilibrium position [40]. Temperature dependence of the thermal expansion coefficient $\alpha$ at fixed pressures for the herein investigated materials is depicted in Fig. 5. From Fig. 5, one can see that $\alpha$ increases sharply with the increasing temperature (with $T^3$) below 200 K ($T < 200$ K) then gradually approaches to a linear increase for $T > 200$ K and the propensity of increment becomes moderate. Pressure is also an important influencing factor on the thermal expansion $\alpha$. From Fig. 5, we can note also that at a fixed temperature $T$ the thermal expansion $\alpha$ decreases exponentially with increasing pressure. So, there is a
large thermal expansion at low pressure which is in accordance with the variation of volume with pressure, as shown in Fig. 3(b). The increasing temperature dependence of the thermal expansion $\alpha$ is as important as the decreasing pressure dependence of the volume thermal expansion coefficient $\alpha$. At high temperatures and high pressures, the thermal expansion coefficient $\alpha$ would converge to a constant value. Values of the thermal expansion $\alpha$ at zero pressure and 300 K for all herein studied materials are summarized in Table 4.

Variation of the Debye temperature $\Theta_D$ with temperature at some fixed pressures (for clarity only at two different pressures) for the YS, YSe and YTe compounds in both phases B1 and B2 are shown in Fig. 6(a). It can be seen that $\Theta_D$ is nearly constant from 0 to 100 K and then it decreases almost linearly with the
increasing temperature. From Fig. 6(a) one can see that as the pressure goes higher, the decreased magnitude of $\Theta_D$ becomes small. The volume dependence of the Debye temperature $\Theta_D$ is shown in Fig. 6(b) at some fixed temperatures. All points lie on a single curve, demonstrating both the consistency of our calculations and the fact that the Debye temperature is a function of the volume only, in accordance with the quasi-harmonic approximation and the simplification given by Eq. (3). It is noted that as the volume $V$ increases, the value of the Debye temperature decreases. The relatively small effect of the temperature on the Debye temperature can be explained by the small effect on the volume changes. It is observed that for constant temperature the Debye temperature of the herein studied materials increases almost linearly with the decrease of the unit cell volume.

The mechanical softening as evident from volume dependent Debye temperature behavior in YX (X=S, Se, and Te) is attributed to YY, XX, and YX bond elongation due to lattice vibration. The temperature dependent Debye temperature curve in YX documents a decreasing trend with enhanced temperature. The outcome is the thermal softening of lattice results from YY, XX, and YX bond expansion and bond weakening due to thermal stress. To our knowledge this is the first quantitative theoretical prediction of the high pressure and high temperature dependence elastic and thermal behavior of YX monochalcogens (X=S, Se, and Te) and still awaits experimental confirmations. We note here that at the phase transition pressures $P_T$ and zero temperature, the Debye temperature $\Theta_D$ is equal to 681.9, 493.05 and 344.67 K for the YS, YSe and YTe compounds, respectively, in the B1 structure, and it is equal to 657.18, 477.36 and 343.35 K, respectively, in the B2 structure. Values of the Debye temperature $\Theta_D$ at zero pressure and 300 K for all herein studied materials are summarized in Table 4.

Knowledge of the isochoric heat capacity $C_V$ of materials does not only provide a fundamental insight into their vibrational properties but is also mandatory for many applications. At intermediate temperatures, temperature dependence of the heat capacity $C_V$ is governed by the details of the vibrations of atoms and has been able to be determined only experimentally for a long time past. Fig. 7 illustrates the temperature dependence of the isochoric heat capacity $C_V$ and isobaric heat capacity $C_P$ for B1 and B2 phases of the herein studied ytterbium-chalcogenides YX (X=S, Se, Te) at two different temperatures. It is readily seen that when $T < 400$ K, the heat capacities $C_V$ and $C_P$ are strongly dependent on the temperature and pressure which is attributed to the anharmonic approximation of the Debye model. However, at higher pressures and/or higher temperatures, the anharmonic effect on $C_V$ and $C_P$ is suppressed, and $C_P$ follows a linear increase, whereas $C_V$ tends to the Dulong–Petit limit ($\approx 50$ J mol$^{-1}$ K$^{-1}$). We note that at a given temperature, $C_V$ and $C_P$ values of the B1 phases of the ytterbium-chalcogenides YX are larger than that of their B2 phases. We have reported in Fig. 7 the existing experimental results of the $C_P$ of the B1 phase of YS for the sake of comparison; the agreement is overall good between the present results and the experimental measurement up to 500 K, then our calculated values of $C_P$ tends to become increasingly smaller than the measured ones [41]. Values of the heat capacities $C_V$ and $C_P$ at zero

<table>
<thead>
<tr>
<th>YS</th>
<th>$C_V$ (J mol$^{-1}$ K$^{-1}$)</th>
<th>$C_P$ (J mol$^{-1}$ K$^{-1}$)</th>
<th>$\alpha$ (10$^{-5}$ K$^{-1}$)</th>
<th>$\Theta_D$ (K)</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Fm\bar{3}m$</td>
<td>45.4</td>
<td>46.5</td>
<td>3.7</td>
<td>412.9</td>
<td>2.0</td>
</tr>
<tr>
<td>Expt. [41]</td>
<td>46.42</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$Pm\bar{3}m$</td>
<td>45.9</td>
<td>46.42</td>
<td>4.3</td>
<td>389.0</td>
<td>1.9</td>
</tr>
<tr>
<td>YSe</td>
<td>$Fm\bar{3}m$</td>
<td>47.0</td>
<td>48.2</td>
<td>4.1</td>
<td>327.0</td>
</tr>
<tr>
<td>$Pm\bar{3}m$</td>
<td>47.3</td>
<td>48.6</td>
<td>4.6</td>
<td>310.6</td>
<td>1.9</td>
</tr>
<tr>
<td>YTe</td>
<td>$Fm\bar{3}m$</td>
<td>47.9</td>
<td>49.2</td>
<td>4.3</td>
<td>264.5</td>
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<tr>
<td>$Pm\bar{3}m$</td>
<td>47.9</td>
<td>49.3</td>
<td>4.5</td>
<td>267.4</td>
<td>2.0</td>
</tr>
</tbody>
</table>

Fig. 6. Variation of the Debye temperature $\Theta_D$ with the unit cell volume at zero temperature for the YS, YSe and YTe compounds in both B1 and B2 phases.
pressure and 300 K for all herein studied materials are summarized in Table 4.

Finally, we turn to the temperature dependence of the single-crystals elastic constants $C_{ij}$ and polycrystalline elastic moduli. First, equilibrium volumes at various temperatures are determined from the quasi-harmonic Debye approximation. Second, we calculated the isothermal elastic constants $C_{ij}(V)$ at these different volumes using the method developed and implemented in Wien2K code [7]. The combination of temperature dependence of the volume $V(T)$ and volume dependence of the elastic constants $C_{ij}(V)$ leads to the temperature dependence of elastic constants $C_{ij}$. In general, the elastic moduli of solid soften with increasing temperature due to the thermal expansion. The evolution of the elastic constants, $C_{11}$, $C_{44}$ and $C_{12}$, as function of temperature for all herein considered materials at zero pressure is depicted in Fig. 8. We note here that we are not aware of any experimental measurements or theoretical calculations of the temperature dependence of the elastic properties in these materials.

Fig. 7. Variation of the heat capacity at constant volume $C_v$ (a) and heat capacity at constant pressure $C_p$ (b) with temperature at different fixed pressure for the YS, YSe and YTe compounds in both B1 and B2 phases. Comparison with experimental values for the $C_p$ of YS [25].

Fig. 8. Calculated temperature dependence of the isothermal elastic constants $C_{ij}$ for the YS, YSe and YTe compounds in both B1 and B2 phases. The symbols are the calculated data and the solid lines are second-order polynomial fit.
The considered elastic constants decrease smoothly and monotonically with increasing temperature. \( C_{44} \) and \( C_{12} \) are less sensitive to the temperature variation compared to \( C_{11} \). This behaviour of \( C_{44} \) and \( C_{12} \) versus temperature indicates that temperature will not cause obvious variation of these materials to the shear deformation. The \( C_{ij} \)-temperature data are fitted to a second-order polynomial: \( C_{ij}(T) = C_{ij}(0) + a_i T + b_i T^2 \). The values of the first-order coefficient \( a \) and second-order coefficient \( b \) for all herein studied materials are summarized in Table 5. All calculated elastic constants as function of temperature \( C_{ij}^{T} \) are positive and satisfy the generalized criteria for mechanically stable crystals [26]:

\[
(C_{11}^{T} - C_{12}^{T}) > 0; (C_{11}^{T} + 2C_{12}^{T}) > 0; C_{44}^{T} > 0
\]

Using the obtained temperature dependence of the single-crystal isotherm elastic constants, we have calculated temperature dependences of the isotherm polycrystalline elastic constants, \( B' \), \( C' \) and \( E' \), for the herein studied ytterbium-chalcogenides \( YX \) \((X=\text{Se}, \text{Te})\) in both phases B1 and B2 via Eqs. (12)-(14), they are summarized in Table 6. The adiabatic polycrystalline elastic moduli, \( B' \), \( C' \) and \( E' \), are calculated using the following relations:

\[
B' = B(1 + \alpha T) \quad (16)
\]
\[
C' = C = G_{ii} \quad (17)
\]
\[
E' = \rho E'_{\text{CT}}(\rho C_{\text{Dp}} - E' T^2) \quad (18)
\]

here \( \rho \) is density of mass. The obtained values for the adiabatic polycrystalline elastic moduli, \( B' \), \( C' \) and \( E' \), are also given in Table 6. From Table 6, one can see that both isothermal and adiabatic elastic moduli \((B', B', E', E', G_{ii})\), for \( YX \) compounds, decrease as the temperature increases which means that the thermal effects hardly change elastic moduli. We note that when shear and Young’s modulus decrease with increasing temperature, the \( YS \), \( YSe \) and \( YTe \) compounds became less stiff at high temperature and less resistant to reversible deformation upon shear stress; they became more easily to compress and lengthen.

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### 4. Conclusions

In the present work, using the FP-LAPW method and quasi-harmonic Debye model, we have investigated the structural, thermodynamic and elastic properties of the \( YS \), \( YSe \) and \( YTe \) compounds. First, we have calculated the static structural properties (equilibrium lattice constant, bulk modulus and its derivative), which are in good agreement with the existing data in the literature. Second, we have determined the thermodynamic properties such as heat capacity \( (C_{V}, C_{p}) \), thermal expansion \( \alpha \) and Debye temperature \( \Theta_D \) under high pressure and temperature effects. Our estimated values of heat capacity \( C_{p} \) for \( YS \) at room temperature are in good agreement with the experimental data. The shape of the calculated \( C_{p}(T) \) curve is in good concordance with that one experimentally obtained; which means that the Debye model can accurately estimate the thermodynamic properties of the herein considered compounds. Finally, we have focused our intention on the temperature dependence of the elastic constants. We have found that thermal effects are very significant on the elastic constants. We have found that the \( YS \), \( YSe \) and \( YTe \) compounds became less resistant to reversible deformation upon shear stress and less stiff at high temperature. Our analysis of the predicted elastic moduli shows that the herein studied materials are relatively soft materials with high compressibility, behave in a ductile manner, and characterized by a strong elastic anisotropy. Lastly, we would like to point out that the present work provides for the first time some new data on the temperature dependence of the structural, elastic and thermodynamic properties of the \( YX \) compounds.
References