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Structural elastic and thermodynamic properties of cubic CsCl type MgCa using ab initio approach

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The CsCl-structured MgCa intermetallic compound was examined through computational quantum mechanics, employing DFT methodology via CASTEP implementation. Analysis of volumetric energy correlations revealed fundamental parameters: a 3.868 Å lattice dimension, 27.99 GPa compressibility factor, and corresponding pressure coefficient of 3.70. The LDA framework produced crystallographic and mechanical flexibility values consistent with previously published computational findings. Thermophysical behavior was quantified using Debye quasi-harmonic approximations spanning thermal conditions (0–800 K) and compression states (0–10 GPa). Under standard reference conditions (P = 0 GPa, T = 0 K), the characteristic vibrational temperature parameter reached 319.23 K, exhibiting remarkable concordance with the independently calculated elastic-based estimate of 321.1 K.

Keywords MgCa intermetallic compound, DFT, Ab-initio calculations, Elastic constants, Structural and thermodynamic properties.

Magnesium-based binary alloys are highly promising materials for various applications, including microstructure engineering, the automotive sector, and aerospace industries[1]. Magnesium (Mg) is well known for being an exceptionally lightweight metal, with a density and mechanical properties comparable to natural bone. This characteristic makes it advantageous for biomedical applications, particularly in promoting new bone tissue growth while reducing stress shielding effects commonly associated with conventional metallic implants[2]. The Mg-Ca system has been studied theoretically by Zhou and Gong[2] using first-principles calculations based on density functional theory (DFT) within the generalized gradient approximation (GGA). Their findings indicate that the MgCa compound undergoes a structural transformation from the body-centered cubic (BCC) phase to the hexagonal close-packed (HCP) phase at a pressure of 10.66 GPa. Groh[3] developed interatomic potentials for both pure calcium (Ca) and the Mg–Ca binary system and employed the second nearest-neighbor modified embedded-atom method (MEAM) to calculate their elastic constants, thermal properties, and other physical parameters across different phases. Daoud et *al.*[4] utilized the pseudopotential plane-wave (PP-PW) approach within the DFT framework to study the impact of high pressure (up to 16 GPa) on the structural parameters and elastic properties of the MgCa intermetallic compound in the cubic CsCl-type (B2) structure. Their results revealed a significant deviation from the Cauchy condition, indicating the presence of strong non-central many-body interactions in the (B2) MgCa compound. Additionally, Rekab-Djabri et *al.*[5] investigated the ground-state parameters, elastic properties, and electronic structure of the Mg_3Ca intermetallic compound. They examined its structural behavior in various phases, including Cu_3Au ($L1_2$), $AlFe_3$ ($D0_3$), αReO_3 (B09), and $CuTi_3$ (L60) structures. Their findings showed that under compression, Mg_3Ca transitions from the $D0_3$ to the $D0_9$ phase at

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a pressure of 29.96 GPa using LDA and at 25.1 GPa using GGA. This study aims to investigate the structural, mechanical, and thermodynamic properties of the studied compound using ab initio calculations based on DFT. The analysis of its mechanical and thermal stability helps assess its potential for various technological applications of the MgCa intermetallic compound in the cubic CsCl-type structure. The obtained results offer promising prospects for integrating this material into devices requiring high structural and thermal resistance. Moreover, they provide a valuable reference for future experimental research. This work can thus contribute to the optimization of materials used in electronics, protective coatings, and high-performance alloys.

Calculation method

Our computational framework utilized DFT methodology via the CASTEP implementation[6], employing plane-wave pseudopotential techniques. Exchange-correlation effects were addressed through CA-PZ functional LDA approximations[7,8], while ultrasoft pseudopotentials characterized electron-ion interactions[9]. The numerical parameters included a 450 eV energy cutoff for plane-wave expansion and Brillouin zone sampling across a $16\times16\times16$ Monkhorst-Pack grid[10]. Convergence thresholds encompassed $5\times10-6$ eV/atom for energy differential, alongside specified geometric constraints (0.02 GPa, $5\times10-4$ Å, and 0.01 eV/Å for forces). Thermophysical behavior was investigated utilizing quasi-harmonic Debye approximations[11] across compression states (0–10 GPa) and thermal conditions (0–800 K). Given the absence of experimental measurements for CsCl-structured MgCa, this investigation provides computational predictions of fundamental physical properties through quantum mechanical calculations.

Results and discussion

Equilibrium structural

The intermetallic MgCa compound exhibits cubic crystallization with the CsCl structural arrangement. This configuration features equivalent dimensional parameters along all axes (a = b = c) and right-angled intersections ($\alpha=\beta=\gamma=90°$). Each fundamental crystallographic unit incorporates a single magnesium atom and one calcium atom. Researchers typically derive equilibrium structural characteristics by analyzing the correlation between volumetric variations and total energy states[12,13].

From Fig. 1, which depicts the total energy E_{Tot} as a function of volume V, the static structural parameters can be determined. Specifically, the lattice constant (a_0) is obtained from the volume corresponding to the minimum total energy (E_0). Additionally, the (B_0) and B_0' are extracted by fitting by (BM-EOS) equation, which is given by[14,15]:

$$E(V)-E_0=\frac{9V_0B_0}{16}\left\{B_0'\left[\left(\frac{V_0}{V}\right)^{2/3}-1\right]^3+\left[\left(\frac{V_0}{V}\right)^{2/3}-1\right]^2\left[6-4\left(\frac{V_0}{V}\right)^{2/3}\right]\right\} \quad (1)$$

The Birch-Murnaghan equation of state incorporates both B_0 (the bulk modulus) and its pressure derivative B_0' as fundamental parameters characterizing the material's response to compression. The pressure derivative of the bulk modulus at zero pressure, mathematically defined as: $B_0'=\frac{\partial B}{\partial P}$ at $P=0$. This parameter describes how the bulk modulus changes with pressure at the equilibrium state.

The obtained values of a_0, B_0 and B_0' as well as the minimum total energy E_0 for MgCa intermetallic compound are summarized in Table 1.

These parameters have also been analyzed and compared with other theoretical results, showing strong agreement. For instance, the difference between our lattice constant (3.868 Å) and the theoretical value (3.96 Å) is less than 2.4%[2]. Similarly, our bulk modulus value (27. 99 GPa) deviates by approximately 9.75% from the theoretical value (25.26 GPa). Additionally, our calculated pressure derivative of the bulk modulus (B_0'=3.70) is slightly lower than the theoretical value (4.05) reported by Daoud et *al.*[4]. It is worth noting that the LDA approach generally predicts lower equilibrium lattice constants than the GGA method.

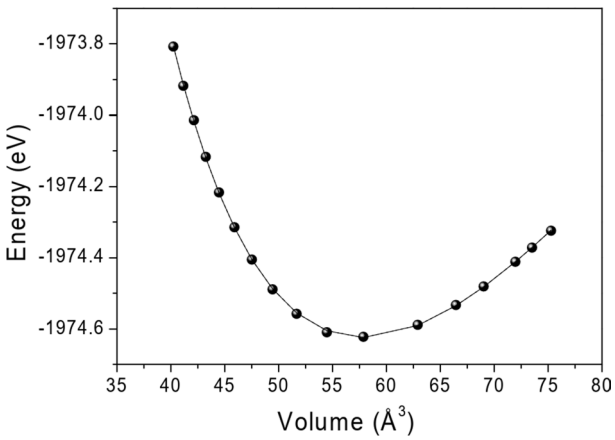

Fig. 1. Plot of the total energy versus the volume of primitive unit cell for CsCl-type structure MgCa.

Parameter	a_0(Å)	B_0 (GPa)	B'_0	E_0 (eV)
This work (DFT-LDA)	3.868	27.99	3.70	−1974.62
Ref. [2] DFT-GGA	3.96	25.26	–	–
Ref. [3] MEAM	3.96	25.16	–	–
Ref. [4] DFT-GGA	3.9764	23.33	4.05	–

Table 1. Equilibrium structural parameters a_0 (Å), bulk modulus B_0(GPa), its pressure derivative $B\prime_0$ and total energy E_0(eV) for (B2) MgCa, in comparison with the theoretical data existing in the literature[2–4].

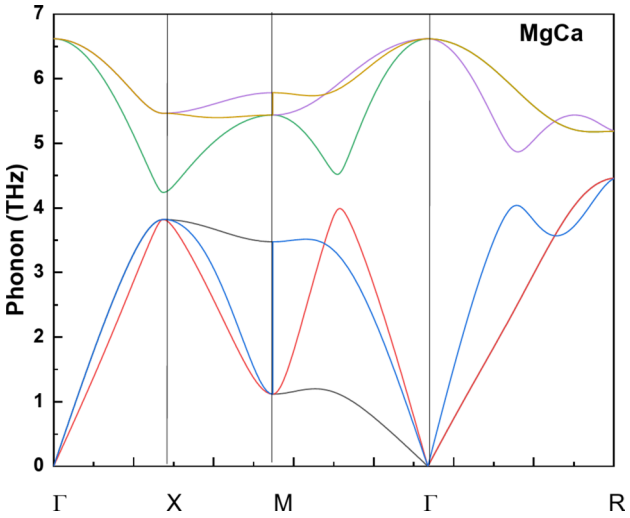

Fig. 2. Phonon dispersion curve of the MgCa compound along the Brillouin zone for (B2) MgCa.

Parameter	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)
This work (DFT-LDA)	38.25	23.80	28.07	28.62
Ref. [2] DFT-GGA	32.28	21.75	24.94	25.26
Ref. [3] MEAM	39.74	18.59	21.61	25.64
Ref. [4] DFT-GGA	37.60	19.82	25.73	25.75

Table 2. Elastic constants C_{ij}(GPa) and aggregate bulk modulus B (GPa) for MgCa.

Moreover, the melting point T_m is correlated with other physical parameters, particularly the bulk modulus B, for cubic-structured solids. It follows the empirical relation B: T_m (K) = 9.3×B (K/GPa) + 607 (K)[16]. By substituting our bulk modulus value (B_0 = 27.99GPa) into this equation, we estimate the melting point of the MgCa intermetallic compound to be 867.3 K. This figure is little more than the 775 ± 300 K theoretical prediction. To our knowledge, no experimental data on the melting point of MgCa intermetallic compounds is available in the literature. Figure 2 illustrates the phonon dispersion curve of the MgCa compound along the Brillouin zone.

The absence of imaginary frequencies confirms the dynamical stability of the cubic CsCl-type phase, which allows for the investigation of the elastic and thermodynamic properties of the compound, especially in the absence of experimental results for this structure.

Elastic properties

The elastic constants are essential for understanding the mechanical properties of materials[17]. For cubic crystals, the bulk modulus Bmay be obtainedfrom the elastic constants C_{ij} as follows: $B = (2C_{12} + C_{11})/3$. Our calculated values of the elastic constants C_{ij} and the bulk modulus for (B2) MgCa are summarized in Table 2. The value 28.62 GPa of the bulk modulus B obtained from the elastic constants is in excellent agreement with the value 27.99 GPa obtained from the fit of the (E-V) data by the BM-EO (Eq. 1). The discrepancy on the bulk modulus B between these two values is only 2.2%. Furthermore, our values of the elastic constants C_{ij} as well as that of the bulk modulus B are in reasonable agreement in comparison with other data existing in the literature.Note that the LDA approach gives higher values for theelastic constants C_{ij} and the bulk modulus than the GGA ones.

The thermodynamic properties of MgCa were investigated using the quasi-harmonic Debye model, which allows us to determine the temperature and pressure dependencies of key physical parameters. This model is based on the G(T, P), which is related to the Helmholtz free energy F(T, V) as follows:

$$PV + F(T,V) = G(T,P) \tag{2}$$

where F(T, V) is expressed as:

$$F_{vib}(T,V) + E_{tot}(V) = F(T,V) \tag{3}$$

Here, $E_{tot}(V)$ is the total energy obtained from DFT calculations, while the vibrational contribution to the free energy, $F_{vib}(T, V)$ is calculated using the Debye approximation:

$$F_{vib}(T,V) = 9k_BT\left[\frac{\theta_D}{8T} + \ln\left(1 - e^{\frac{\theta_D}{T}}\right) - D\frac{\theta_D}{T}\right] \tag{4}$$

The Debye temperature θ_D is a key fundamental parameter in solid-state physics, which is closely associated with various physical properties, including melting temperature, specific heat and elastic constants[17,18]. At above θ_D, the thermal vibrations become more important than the quantum effects conducting that the crystal behaves classically[19,20]. At low temperatures, vibrational excitations are primarily due to acoustic modes. The Debye temperature calculated from elastic constants at low temperatures is identical to that determined from specific heat measurements. The Debye temperature θ_D was deduced from the speed of the sound v_m as follows:

$$\theta_D = \frac{h}{k_B}\left(\frac{3}{4\pi V_a}\right)^{1/3}\nu_m \tag{5}$$

where h is the Plank's constant, V_a is the atomic volume and k_B is the Boltzmann's constant.

The average sound velocity v_m is given by[21,22]:

$$v_m = \left[\frac{1}{3}\left(\frac{2}{{v_t}^3} + \frac{1}{{v_l}^3}\right)\right]^{-1/3} \tag{6}$$

where ν_l and ν_t are the longitudinal and transverse sound velocity, respectively. They are calculated from the following equations:

$$v_l = \left(\frac{3B + 4G}{3\rho}\right)^{1/2} and\, v_t = \left(\frac{G}{\rho}\right)^{1/2} \tag{7}$$

Using the values of the elastic constants C_{ij} obtained in this study for the studied material, the computation yielded average value of the shear modulus G = 16.38 GPa. The average shear modulus (G) was calculated using the Voigt-Reuss-Hill (VRH) homogenization scheme, which is the arithmetic mean of the Voigt and Reuss bounds. For cubic crystals, the Voigt bound (G_V) and Reuss bound (G_R) are calculated through the following relations:

$$G_{\mathrm{V}} = (\mathrm{C}_{11} - \mathrm{C}_{12} + 3\mathrm{C}_{44})/5 \tag{8}$$

$$G_{\mathrm{R}} = \frac{5(\mathrm{C}_{11} - \mathrm{C}_{12}) \times \mathrm{C}_{44}}{4 \times \mathrm{C}_{44} + 3(\mathrm{C}_{11} - \mathrm{C}_{12})} \tag{9}$$

Therefore, the average shear modulus according to the VRH scheme is:

$$G = \frac{G_{\mathrm{V}} + G_{\mathrm{R}}}{2} \tag{10}$$

The calculated of the ρ, v_l, v_t, v_m and θ_D for CsCl-type structure MgCa intermetallic compound are given in Table 3.

All the elastic constants C_{ij} obtained in this work are slightly higher than the theoretical ones reported by Daoud et al.[4], one can notice that the calculated values of the sound velocities (v_l, v_t and v_m) and the Debye temperature θ_D for MgCa are slightly lower than their theoretical ones. The percentage deviation is around 5.16% for v_m; while the discrepancy on θ_D is only around 2.35%.Note that the LDA approach gives higher values for v_l, v_t, v_t, ρ and θ_D than the GGA onesin the case M_2XC (M = Cr and Ti, X = Al and Ga) ternary compounds[17].

Thermodynamic properties

The thermodynamic properties are essential parameters for studying chemical reactivity and crystal stability[23,24]. Pressure is a fundamental thermodynamic variable that can be used to transfer matter from one state to another.

Parameter	ρ (g/cm^3)	ν_l (km/s)	ν_t (km/s)	ν_m (km/s)	θ_D (K)
This work (DFT-LDA)	1.844	5.231	2.980	3.313	321.1
Ref. [4]DFT-GGA	1.700	5.323	3.145	3.484	328.65

Table 3. Mass density, longitudinal v_l, transversal v_t and average v_m sound velocities and Debye temperature θ_D for MgCa.

The effect of pressure (0, 2, 4, 6, 8 and 10 GPa) and temperature on the unit cell volume for MgCa is presented in Fig. 3(a, b). Notice that theunit cell volume decreases with compression at (0, 300, 600 and 800 K). The bond length is decreasing, which causes the volume to shrink under the compression action. In other hand, the elevation of temperature conducts to an expansion of the bond-length. Similar behavior has been observed for different materials such as for cubic zinc-blende AlP, for copper scandium (CuSc) intermetallic compound and for (B3) boron nitride (*c*-BN) compound[25] at temperatures 300, 600 and 900 K andin the pressure range 0 to36 GPa.

At temperatures of 0, 300, 600 and 800 K, the fits of the unit cell volume *V*values for MgCa intermetallic compound obey the following quadratic expressions, respectively:

$$V = 58.29 - -1.78p + 6.20 \times 10^{-2}p^2 \tag{11}$$

$$V = 59.52 - -1.97p + 7.20 \times 10^{-2}p^2 \tag{12}$$

$$V = 61.63 - -2.30p + 8.96 \times 10^{-2}p^2 \tag{13}$$

$$V = 63.35 - -2.58p + 10.06 \times 10^{-1}p^2 \tag{14}$$

where the unit cell volume V is expressed in $Å^3$ and the pressure is expressed in GPa.

According to the laws of thermodynamics, the isothermal bulk modulus B_T may be obtained from the following formula[11]:

$$B_T = -V\left(\frac{\partial p}{\partial V}\right)_T \tag{15}$$

Figure 4 shows the isothermal bulk modulus B_T for CsCl-type structure MgCa versus pressure and temperature. It increases with increasing pressure and decreases with increasing temperature. Similar behavior has been observed for AlP semiconducting compound, for copper scandium (CuSc) intermetallic compound at temperatures 0, 300, 600 and 1000 K and pressure ranging from 0 to 12 GPa, for *c*-BN binary compound, for Co_2MnAl, Co_2MnGe and Co_2MnSn ternary compounds[26] and forthe ordered $Ge_{0.5}Sn_{0.5}$ in cubic zinc-blende phase[27].

The pressure derivative of the isothermal bulk modulus B_T' is given by the following formula[11]:

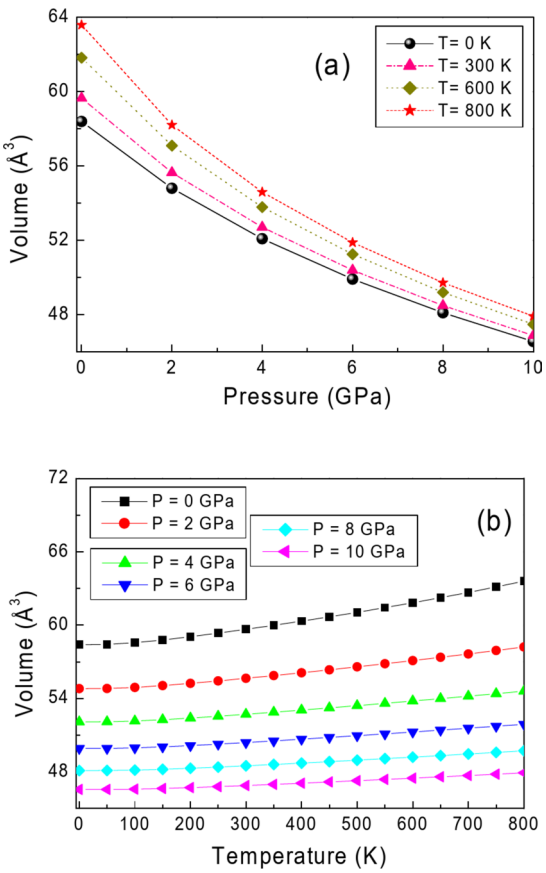

Fig. 3. Effect of pressure and temperature on unit cell volume for CsCl-type structure MgCa intermetallic compound.

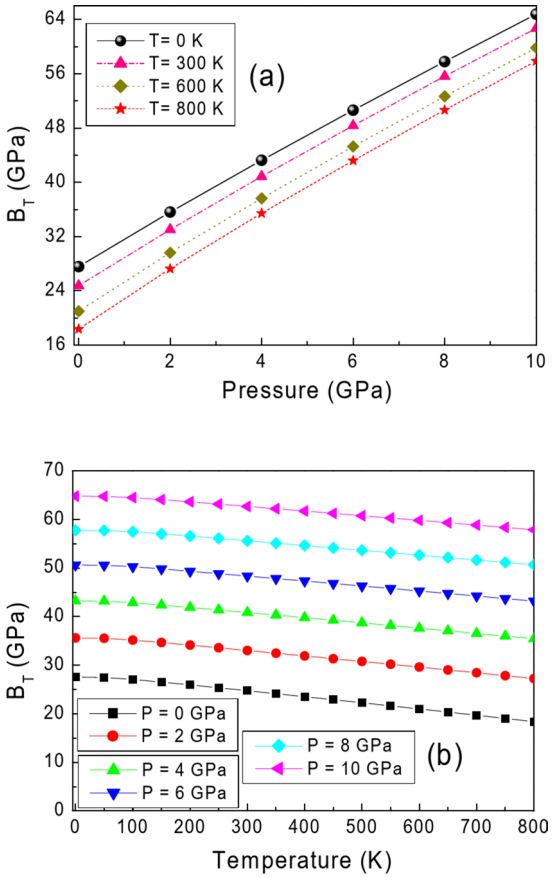

Fig. 4. Isothermal bulk modulus B_T for CsCl-type structure MgCa versus pressure and temperature.

$$B'_T = (\partial B_T/\partial p)_T \tag{16}$$

The variation of $B_T'(p, T)$ as a function of compression at different temperatures (0, 300, 600 and 800 K) and versus temperature at different pressures (0, 2, 4, 6, 8 and 10 GPa) for MgCa are displayed in Fig. 5(a, b). We observe that $B_T'(p, T)$ decreases as pressure enhances and increases with the augmentation of 0 to 800 K. At $p = 10$ GPa, $B_T'(p, T)$ changes slowly with arising of the temperature. The value 4.15 of $B_T'(p, T)$ obtained at $p = 0$ and $T = 0$ K is slightly higher than that 3.70 of B_0' obtained from the fit with Eq. (1).

The following quadratic expressions are the different fits on B_T' as a function of temperature (in K) at 0, 2, 4, 6, 8 and 10 GPa, respectively:

$$B_T\prime = 4.15 + 4.21 \times 10^{-4}\mathrm{T} + 3.36 \times 10^{-7}\mathrm{T}^2 \tag{17}$$

$$B_T\prime = 3.90 + 30.06 \times 10^{-4}\mathrm{T} + 1.30 \times 10^{-7}\mathrm{T}^2 \tag{18}$$

$$B_T\prime = 3.74 + 2.29 \times 10^{-4}\mathrm{T} + 0.69 \times 10^{-7}\mathrm{T}^2 \tag{19}$$

$$B_T\prime = 3.63 + 1.75 \times 10^{-4}\mathrm{T} + 0.42 \times 10^{-7}\mathrm{T}^2 \tag{20}$$

$$B_T\prime = 3.54 + 1.33 \times 10^{-4}\mathrm{T} + 0.28 \times 10^{-7}\mathrm{T}^2 \tag{21}$$

$$B_T\prime = 3.47 + 0.99 \times 10^{-4}\mathrm{T} + 0.20 \times 10^{-7}\mathrm{T}^2 \tag{22}$$

In the quasi-harmonic model, the Debye temperature θ_D may be calculated employing the following expression[11]:

$$\theta_D = \frac{\hbar}{k}\left(6\pi^2 V^{0.5} n\right)^{1/3} f(\sigma)\,(B_s/M)^{1/2} \tag{23}$$

where $\hbar$ is the reduced Planck constant, M is the molecular mass per primitive cell, B_S is the adiabatic bulk modulus, k is the Boltzmann constant, $f(\sigma)$ is functional of other quantity σ which is the Poisson ratio.

The variation of θ_D as a function of compression at (0, 300, 600 and 800 K) and versus temperature at (0, 2, 4, 6, 8 and 10 GPa) for MgCa are displayed in Fig. 6(a, b).

As pressure rises, the Debye temperature rises monotonically; conversely, as temperature rises, it falls. At a fixed low value of pressures (0, 2, 4 and 6 GPa), the θ_D decreases with rising temperature for MgCa, while for high

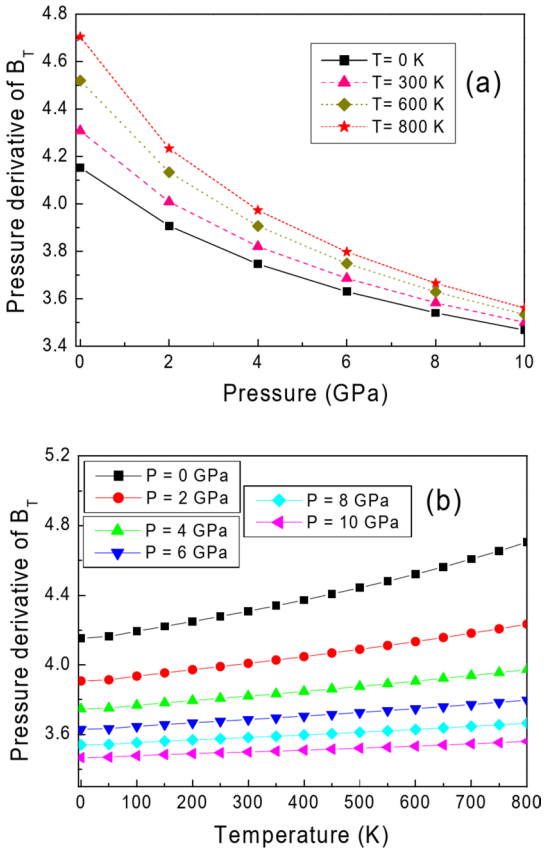

Fig. 5. Effect of pressure and temperature on B_T' for MgCa material.

values of pressure (8 and 10 GPa) the θ_D for MgCa becomes unchanged with rising temperature. An increase in the Debye temperature θ_D with pressure has also been observed for calcium oxide (CaO) compound[28], for cubic rock-salt cadmium oxide (CdO) semiconducting compound[29], for cubic zinc-blende gallium antimonide (GaSb) compound[30], for cubic zinc-blende boron antimonide (BSb) semiconducting compound[31], for cubic perovskite $CsCdF_3$ ternary material[32] and for beta silicon carbide (3 C-SiC)[33]. At $p=0$ and $T=0$ K, our calculation yielded value of the Debye temperature $\theta_D \sim 319.23$ K, which is in excellent agreement with our value 321.1 K obtained from the elastic constants. The discrepancy on θ_D between the two values obtained from the quasi-harmonic Debye model and the elastic constants is less than 0.60%. The following quadratic expressions are the different fits on θ_D as a function of pressure (in GPa) at 0, 300, 600 and 800 K, respectively:

$$\theta_D = 319.97 + 20.14p - 4.92 \times 10^{-1}p^2 \quad (24)$$

$$\theta_D = 307.13 + 21.63p - 5.64 \times 10^{-1}p^2 \quad (25)$$

$$\theta_D = 2860.05 + 23.96p - 6.83 \times 10^{-1}p^2 \quad (26)$$

$$\theta_D = 269.86 + 25.96p - 7.92 \times 10^{-1}p^2 \quad (27)$$

where the volume V is expressed in $Å^3$ and the pressure is in GPa.

The structural behaviour under temperature effect of material may be explicated by the thermal expansion coefficient[34]. The volumetric thermal expansion coefficient$\alpha$was given by the following formula:

$$\alpha = -\frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p \quad (28)$$

where V is the volume, T is the temperature and $p$arethe pressure.

The effect of pressure (0, 2, 4, 6, 8 and 10 GPa) and temperature on the volumetric thermal expansion coefficient for MgCa is presented in Fig. 7 (a, b), respectively.

We observe that the volumetric thermal expansion coefficient α of MgCa decreases with compression and enhances with temperature from 0 to 800 K. The increasing of α with increasing temperature andthe decreasing of α with increasing pressure was observed also for the alkali metal chalcogenide K_2S binary compound, for the perovskite oxide $SnTiO_3$ in the cubic phase[34], for (B2) MgCu material[35] and for the superconductorNb_3Ga intermetallic binary compound[36] at pressures 0, 10, 20, 30 and 40 GPa, and temperature ranging from 0 to

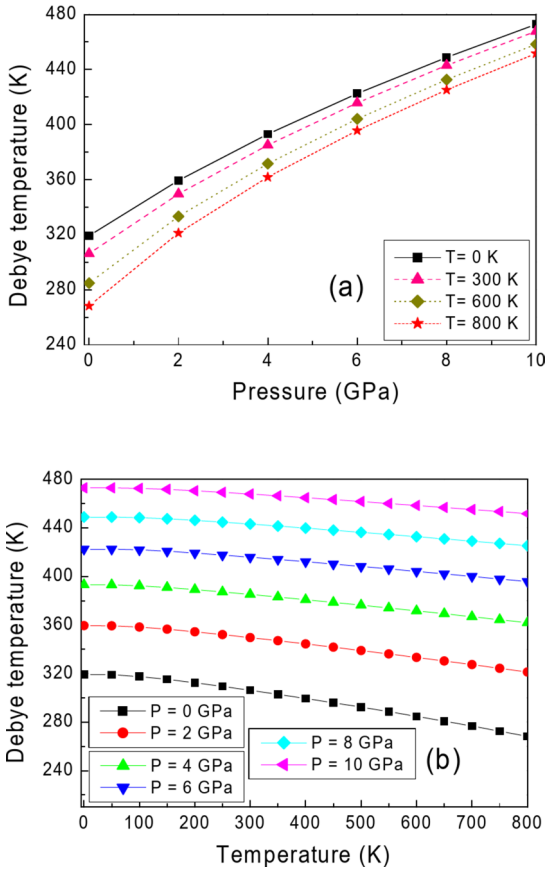

Fig. 6. Impact of pressure at 0, 300, 600 and 800 K and temperature at 0, 2, 4, 6, 8 and 10 GPa on Debye temperature for CsCl-type structure MgCa.

1000 K. At high pressures (8 and 10 GPa) and high temperatures (T > 500 K), the volumetric thermal expansion coefficient changes slowly with arising of the temperature. At ambient pressure the thermal expansion coefficient can represented simply as[37]:

$$a\,(\mathrm{T}) = a + b\mathrm{T} - c/\mathrm{T}^2 \tag{29}$$

For MgCa, the numerical values of the constants *a*, *b* and*c* are found 7.68×10^{-5}/K, 9.35×10^{-8}/K^2 and 1.5×10^{-1} K, respectively.

The constant pressure heat capacity *Cp* was given by the following formula[11]:

$$Cp = \left(\frac{\partial H}{\partial T}\right)_p \tag{19}$$

where *H* is the enthalpy.

The variation of the constant pressure heat capacity *Cp* as a function of pressure at 100, 300, 600 and 800 K for MgCa was illustrated in Fig. 8 (a), while the variation of *Cp* as a function of temperature T at (0, 2, 4, 6, 8 and 10 GPa) was shown in Fig. 8 (b).

We observe that the constant pressure heat capacity *Cp* of MgCa decreases with compression and increases with temperature from 0 to 800 K. The increasing of *Cp* with increasing of temperature and decreasing of *Cp* with increasing pressure was observed also for aluminum phosphide (AlP) binary semiconductor[12], for the alkali metalchalcogenide K_2S binary compound[20] and for CsCl-type structure MgCu binary intermetallic compound[35].

Except the data reported on the entropy*S*and specific heat capacity $C_V$by Daoud et al.[4], we think that there is no data or results reported in the literature on the thermodynamic properties for MgCa with CsCl-type structure structure.

Conclusion

In this study, we investigated the structural parameters and elastic constants of CsCl-type structure MgCa intermetallic compound. We use the plane-wave pseudopotential approach within the DFT. Our calculated

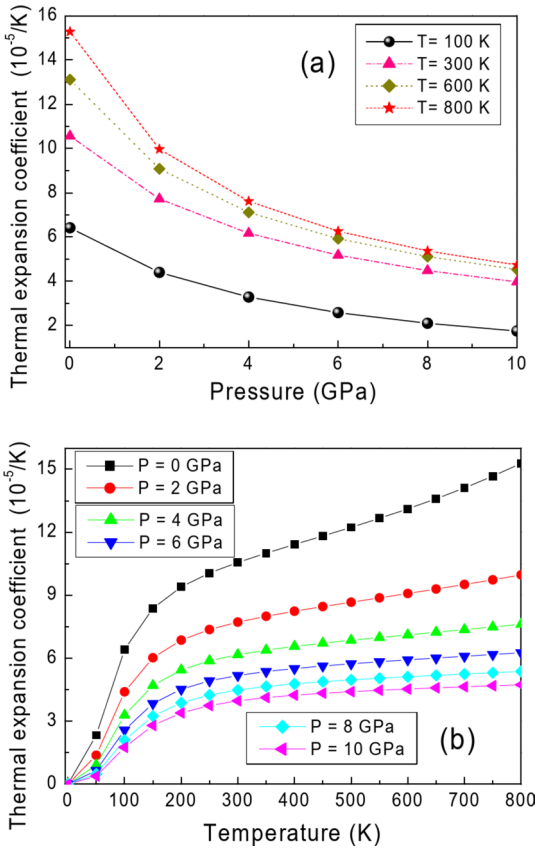

Fig. 7. Impact of pressure at 100, 300, 600 and 800 K and temperature at 0, 2, 4, 6, 8 and 10 GPa on volumetric thermal expansion coefficient for MgCa.

structural parameters and mechanical properties agreed well with other data reported in the literature. The melting temperature T_m of CsCl-type structure MgCa has been also evaluated. Furthermore, the impact of pressure varied within 0 – 10 GPa and temperature varied within 0–800 K on the thermodynamic properties of MgCa have been determined using the quasi-harmonic Debye model. At $p = 0$ and $T = 0$ K, our calculation yielded value of the Debye temperature ~ 319.23 K, which concordsvery well with the value 321.1 K obtained from the elastic constants, while at $p = 0$ and $T = 800$ K, the Debye temperature of CsCl-type structure MgCa reaches the value ~ 268.21 K.

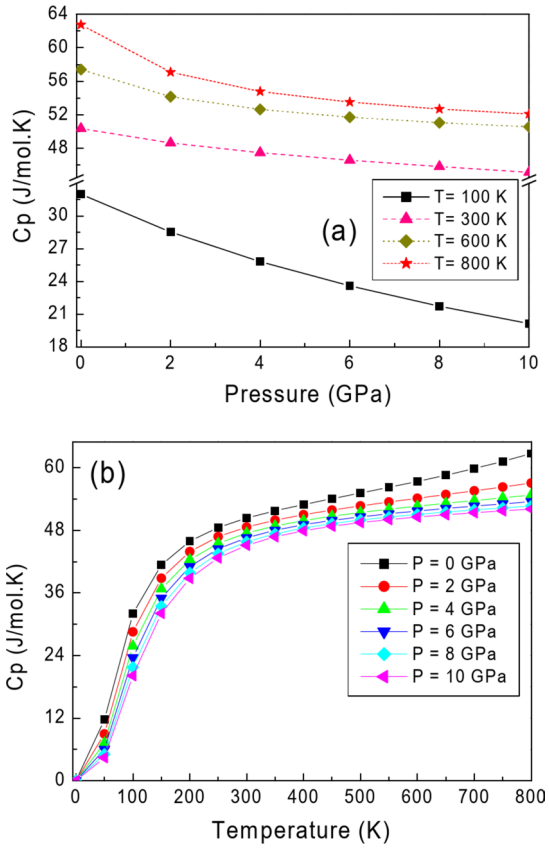

Fig. 8. Plot between heat capacity *Cp* and pressure at various temperatures and between *Cp* and temperature at various pressures for MgCa.

Data availability

Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the author (fatmimessaoud@yahoo.fr) upon reasonable request.

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Declarations

Competing interests

The authors declare no competing interests.

Additional information

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