

Structural and elastic properties of Zr_2AlX and Ti_2AlX ($X = C$ and N) under pressure effect

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Abstract. Using first-principles density functional calculations, the effect of high pressures, up to 20 GPa, on the structural and elastic properties of Zr_2AlX and Ti_2AlX , with $X = C$ and N , were studied by means of the pseudo-potential plane-waves method. Calculations were performed within the local density approximation to the exchange-correlation approximation energy. The lattice constants and the internal parameters are in agreement with the available results. The elastic constants and their pressure dependence are calculated using the static finite strain technique. We derived the bulk and shear moduli, Young's moduli and Poisson's ratio for ideal polycrystalline Zr_2AlX and Ti_2AlX aggregates. We estimated the Debye temperature of Zr_2AlX and Ti_2AlX from the average sound velocity. This is the first quantitative theoretical prediction of the elastic properties of Zr_2AlC , Zr_2AlN and Ti_2AlN compounds, and it still awaits experimental confirmation.

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1 Introduction

Recently, it has become possible to compute with great accuracy an important number of electronic and structural parameters of solids from first-principles calculations. This kind of development in computer simulations has opened many interesting and exciting possibilities in condensed matter studies. For example, it is now possible to explain and predict properties of solids which were previously inaccessible to experiments.

Nowadays, M_2AX phases, where M is an early transition metal, A is a group IIIA or IVA element, and X is either C or N , attract more and more attention due to their unusual properties. They exhibit materials properties that are associated with both metals and ceramics (for details see [1] and the references cited therein). Like metals, they are electrically and thermally conductive, not susceptible to thermal shock, plastic at high temperature and exceptionally damage tolerant, and most readily machinable. Like ceramics, they are elastically rigid, lightweight, creep and fatigue resistant and maintain their strengths to high temperatures [2–12]. This makes them attractive for many applications such as structural materials at elevated temperature. Up to now, more than 50

M_2AX phases have been discovered, among them there are some M_2AlX phases.

The M_2AlX phases with $M = (Ti, V, Cr, Nb, Ta)$ and $X = (N, C)$ have been experimentally and theoretically extensively studied [1–25]. However, there are few studies on Zr_2AlX [26]. The elastic constants are among the properties which are not yet calculated or measured for Zr_2AlC , Zr_2AlN and Ti_2AlN compounds. Moreover, it seems that there are no studies about the strain effect on the structural properties of Zr_2AlX compounds.

Elastic properties of solids are closely related to many fundamental solid-state properties, such as equation of state (EOS), specific heat thermal expansion, Debye temperature, Grüneisen parameter, melting point and many others. From the elastic constants, one can obtain valuable information about the binding characteristics between adjacent atomic planes, the anisotropic character of the bonding and the structural stability.

The behaviour of materials under compression based on calculations or measurements has become an important subject of study in the recent years as it provides insight into the nature of the solid-state theories and determines the values of fundamental parameters [27].

We therefore think that it is worthwhile to perform calculations on the structural and elastic properties of Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN under pressure

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using the ultra-soft pseudo-potential plane-waves (PP-PW) method in order to provide reference data for the experimentalists and to complete existing theoretical works on this fascinating class of materials. To judge the reliability and accuracy of our predicted results for Zr_2AlN , Zr_2AlC and Ti_2AlN , results of Ti_2AlC are compared to the available experimental results.

2 Computational methods

The first-principle calculations are performed by employing pseudo-potential plane-waves (PP-PW) approach based on density functional theory (DFT) [28,29] and implemented in the most recent version of CASTEP (Cambridge Serial Total Energy Package) code [30]. The major advantages of this approach are: the ease of computing forces and stresses; good convergence control with respect to all computational parameters; favourable scaling with number of atoms in the system and the ability to perform fast calculations by neglecting core electrons. The exchange-correlation potential is treated within the LDA, developed by Ceperly and Alder and parameterized by Perdew and Zunger [31,32]. Two parameters that affect the accuracy of calculations are the kinetic energy cut-off which determines the number of plane waves in the expansion and the number of special k -points used for the Brillouin zone (BZ) integration. We performed convergence with respect to BZ sampling and the size of the basis set. Converged results were achieved with $9 \times 9 \times 2$ special k -points mesh [33]. The size of the basis set is given by cut-off energy equal to 280 eV. Careful convergence tests show that with these parameters relative energy converged to better than 5×10^{-7} eV/atom, forces below 0.01 eV \AA^{-1} and total stresses below 0.02 eV \AA^{-3} .

3 Results and discussion

3.1 Structural properties

Zr_2AlX and Ti_2AlX ($X = C, N$) compounds crystallize in the Cr_2AlCd crystal structure, with space group $P6_3/mmc$ (#194). Its unit cell contains two formula units. The X atoms are positioned at the $(0, 0, 0)$ positions, the Al atoms at $(1/3, 2/3, 3/4)$ and the four M ($M = Zr, Ti$) atoms at $(1/3, 2/3, z)$. The structure is thus defined by two lattice parameters, a and c , and the internal structural parameter, z . Figure 1 shows the unit cell of Zr_2AlC as a structural model for the crystalline structure of M_2AX phases ($M = Zr, A = Al$ and $X = C$).

The method used to optimize the structural geometry involves computation of the self-consistent total energy of the system by solution of the Kohn-Sham equations, the forces and stresses, using the Hellman-Feynman theorem, and the subsequent relaxation of the electrons, the ions and the unit cell. The ions were relaxed until the Hellman-Feynman forces were below 0.01 eV \AA^{-1} and the cell parameters were relaxed until total stresses were below 0.02 GPa. The calculated lattice parameters, a_0 and

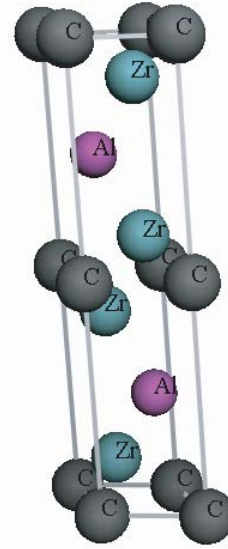


Fig. 1. The unit cell of Zr_2AlC .

c_0 , and the internal structural parameter z , for Zr_2AlX and Ti_2AlX ($X = C, N$) as determined from geometry at $P = 0$ GPa, are given in Table 1 together with the available results of other calculations and experimental data. There is a reasonable agreement between our results and those of the previous calculations and measurements. The slight underestimation of the lattice constants of Ti_2AlC and Ti_2AlN compared to the experimental ones is due to the use of LDA which is known to underestimate the lattice constants.

In order to show how the structural parameters under pressure in these compounds behave, the equilibrium geometries of Zr_2AlX and Ti_2AlX unit cells were computed at fixed values of applied hydrostatic pressure in the range from 0 to 20 GPa with the step of 5 GPa, where, at each pressure, a complete optimization for the structural parameters was performed. Note that it is assumed here that no phase transformations occurred in these systems; it was indeed reported that were no phase transformations observed in Ti_2AlN , Ti_2AlC , V_2AlC , Cr_2AlC , Nb_2AlC , Nb_2AlC and Zr_2InC samples up to pressures ≈ 50 GPa [11, 25,34] by using a synchrotron radiation and a diamond-anvil cell to measure the pressure dependency of the lattice parameters of these compounds. Figure 2 plots the variation of the relative changes of the lattice parameters (a/a_0 , c/c_0 , c/a) and the internal parameter, z , versus applied hydrostatic pressure, P . We clearly observe a quadratic dependence in all curves of these four compounds in the considered range of pressure. The solid curve is a quadratic least-squares fit. The values of the linear and quadratic pressure coefficients of a/a_0 , c/c_0 , c/a and z for these compounds are given in Table 2. In all cases, the contraction with pressure along the c -direction is greater than along the a -direction. Similar results were observed for Ti_2AlC , Ti_2AlN , Ti_2AlV , Ti_2AlCr , Ti_2AlNb and Ti_2AlTa [11,25]. The main difference between the four compounds, however, is obvious in the relative changes

Table 1. Structural parameters of Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN at zero-pressure: lattice constants, a_0 and c_0 , internal parameter, z , bulk modulus, B_0 , and its pressure derivative, B' , along with the previous theoretical and experimental results. The values of B_0 and B' are evaluated from the fitting of the pressure-volume data to an analytical equation of state.

| Compound | | $a_0(\text{\AA})$ | $c_0(\text{\AA})$ | c_0/a_0 | $B_0(\text{GPa})$ | B' | z |
|-----------|-------------|-------------------|-------------------|-----------|-------------------|------|---------|
| Zr_2AlC | Present | 3.26899 | 14.40815 | 4.40753 | 134 | 3.89 | 0.08646 |
| | Theory [26] | 3.2104 | 14.2460 | 4.437 | 176.28 | 4.01 | 0.08693 |
| Zr_2AlN | Present | 3.20753 | 14.16947 | 4.41757 | 156 | 3.97 | 0.08824 |
| | Theory [26] | 3.2155 | 14.2134 | 4.420 | 177.10 | 4.32 | 0.08696 |
| Ti_2AlC | Expt. [10] | | | | 144 | | |
| | Expt. [24] | 3.058 | 13.642 | 4.46108 | | | 0.085 |
| | Theory [24] | 3.07 | 13.74 | 4.47557 | 164 | 4.6 | 0.0835 |
| | Expt. [11] | 3.065 | 13.71 | 4.47308 | 186 | 4.0 | |
| | Expt. [8] | 3.04 | 13.60 | 4.47368 | | | |
| Ti_2AlN | Present | 2.9504 | 13.3954 | 4.54019 | 169 | 4.0 | 0.08515 |
| | Expt. [11] | 2.986 | 13.60 | 4.55459 | 169 | 3.5 | |
| | Expt. [24] | 2.991 | 13.619 | 4.5533 | | | 0.085 |
| | Theory [24] | 3.0 | 13.68 | 4.56 | 175 | 4.6 | 0.0854 |

in the c -direction. The relative changes in the a -direction are almost indistinguishable. Along the c -direction Zr_2AlN (Ti_2AlN) is less compressible than Zr_2AlC (Ti_2AlC), consequently, the anisotropy is greater for the former than for the latter. Another consequence is that the bulk modulus of Zr_2AlC (Ti_2AlC) is slightly lower than that of Zr_2AlN (Ti_2AlN).

Based on the fact that the compressibilities along the a -direction for both Zr_2AlN and Zr_2AlC (Ti_2AlN and Ti_2AlC) are quite similar, it is reasonable to assume that the compressibility along the a -direction is dominated by the Zr-Al (Ti-Al) bonds that are identical in both compounds. Along the c -axis, on the other hand, the main difference between the two compounds must thus be traced to the Zr-X (Ti-X) bonds. The c -lattice parameter of Zr_2AlN (Ti_2AlN) is shorter than that in Zr_2AlC (Ti_2AlC) (Tab. 1), then the Zr-C (Ti-C) bonds are weaker than Zr-N (Ti-C) bonds.

The calculated total energies for different volumes of the unit cell around the equilibrium cell volume V_0 are fitted to the Birch-Murnaghan equation [35]:

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

with $V_0 = 133.34152 \text{ \AA}^3$, 126.24796 \AA^3 , 106.77485 \AA^3 and 100.98513 \AA^3 for Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN respectively, fixed at the value determined from the zero-pressure data. We obtained, by least-squares fitting, the bulk modulus B_0 at zero pressure and its pressure derivative B' . These are listed in Table 1. The calculated bulk modulus values using FP-LAPW method [26] for Zr_2AlC

and Zr_2AlN are slightly higher than our calculated ones. These differences can be attributed to the fact that the authors in reference [26] performed no relaxation of the compressed structures. The obtained results for Ti_2AlN and Ti_2AlC are in good agreement with the experimental ones [10,11].

3.2 Elastic properties

It is well established that first principle studies based on DFT can be used to obtain reliable elastic properties of inorganic compounds [36,37]. Several methods are available for computation of stiffness coefficients, but currently the finite strain method seems to be most commonly used and this one is used in the present work. In this approach, the ground state structure is strained according to symmetry-dependent strain patterns with varying amplitudes and a subsequent computing of the stress tensor after a re-optimization of the internal structure parameters, i.e. after a geometry optimization with fixed cell parameters. The elastic stiffness coefficients are then the proportionality coefficients relating the applied strain to the computed stress, $\sigma_{ij} = C_{ijklm}\varepsilon_{lm}$. Due to the symmetry of the elastic stiffness coefficients tensor \bar{C} the binary notation C_{pg} is used instead the quaternary one C_{ijklm} . The connection between binary and quaternary notation is made by replacing every two digits (ij) or (lm) by one digit p or g : $11 \rightarrow 1$, $22 \rightarrow 2$, $33 \rightarrow 3$, $23 \rightarrow 4$, $31 \rightarrow 5$, $12 \rightarrow 6$. Using the binary notation stress-strain relation become $\sigma_i = C_{ij}\varepsilon_j$. Both stress and strain have three tensile and three shear components, giving six components in total. The linear elastic stiffnesses, C_{ij} , thus form a 6×6 symmetric matrix with a maximum of 21 different components, such that $\sigma_i = C_{ij}\varepsilon_j$ for small stresses σ , and strains, ε [8,39]. Any symmetry present in the structure may make some of these components equal and may

Table 2. Variation of the relative lattice parameters (a/a_0 , c/c_0 , c/a) and internal structural parameter (z) with pressure are described by a quadratic polynomial. The calculated first- (α in 10^{-4} GPa $^{-1}$) and second-order (β in 10^{-5} GPa $^{-2}$) pressure coefficients are listed below for Zr₂AlC, Zr₂AlN, Ti₂AlC and Ti₂AlN, along with the available experimental data.

| | Zr ₂ AlN | | Zr ₂ AlC | | Ti ₂ AlN | | Ti ₂ AlC | |
|------------|---------------------|---------|---------------------|---------|---------------------|---------|---------------------|---------|
| | α | β | α | β | α | β | α | β |
| a/a_0 | | | | | | | | |
| Present | -20.1 | 1.7112 | 22.2 | 1.9924 | -19.0 | 1.637 | -18.8 | 1.0944 |
| Expt. [11] | | | | | -18.0 | 1.0 | -11.08 | 1.0 |
| c/c_0 | | | | | | | | |
| Present | -21.5 | 2.0003 | 27.0 | 3.0971 | -18.6 | 1.4301 | -22.8 | 2.0069 |
| Expt. [11] | | | | | -19.0 | 0.9 | -24.0 | 2.0 |
| c/a | -6.5865 | 1.2391 | -21.2 | 4.6732 | -17.95 | 0.9710 | -18.0 | 3.9963 |
| z | 1.7589 | -0.1766 | 2.4533 | -0.2673 | 1.7896 | -0.18 | 2.848 | -0.2597 |

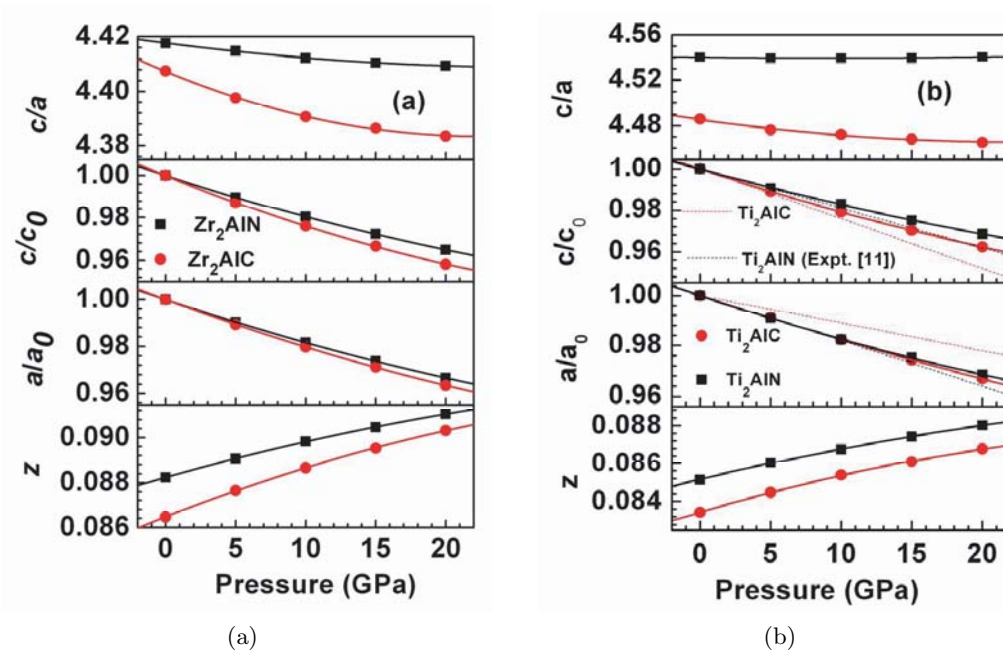


Fig. 2. Pressure dependence of the relative lattice parameters (a/a_0 , c/c_0 , c/a) and internal structural parameter (z) for Zr₂AlC, Zr₂AlN, Ti₂AlC and Ti₂AlN compounds. The solid lines are least-square fits of the data points to a quadratic polynomial. The dashed lines are least-square fits of the experimental data points to a quadratic polynomial [11].

lets other components vanish. A hexagonal crystal has six different symmetry elements (C_{11} , C_{12} , C_{13} , C_{33} , C_{44} , and C_{66}), and only five of them are independent since $C_{66} = (C_{11} - C_{12})/2$. Two different strain patterns, one with non-zero first and fourth components, and another with a non-zero third component, give stresses related to all five independent elastic coefficients for the hexagonal system [40–42]. Two positive and two negative amplitudes were used for each strain component with the maximum value of 0.3%, and then the elastic stiffness coefficients were determined from a linear fit of the calculated stress as a function of strain. One of the strain patterns reduces the cell symmetry; in this case atomic positions were optimized until the forces were below 0.002 eV \AA^{-1} .

In Table 2, we listed the calculated values of the elastic constants C_{ij} . Note that the difference between C_{11} and C_{33} is comparatively small. From Tables 1 and 4, we can see that the calculated value of the bulk modulus B_0

from the elastic constants has nearly the same value as the one obtained from the EOS fitting. This might be an estimate of the reliability and accuracy of our calculated elastic constants for Zr₂AlC, Zr₂AlN, Ti₂AlC and Ti₂AlN compounds. We are not aware of any experimental data on the elastic properties. Future experimental measurements will test our calculated predictions.

Once the elastic constants are determined, we would like to compare our results with experiments, or predict what an experiment would yield for the elastic constants. A problem arises when single crystal samples cannot be obtained. Then it is not possible to measure the individual elastic constants C_{ij} . Instead, the isotropic bulk modulus B and shear modulus G are determined [43]. These quantities cannot in general be calculated directly from the C_{ij} , but we can use our values to place bounds on the isotropic moduli. Reuss found lower bounds for all lattices [44], while Voigt discovered upper bounds [45]. We

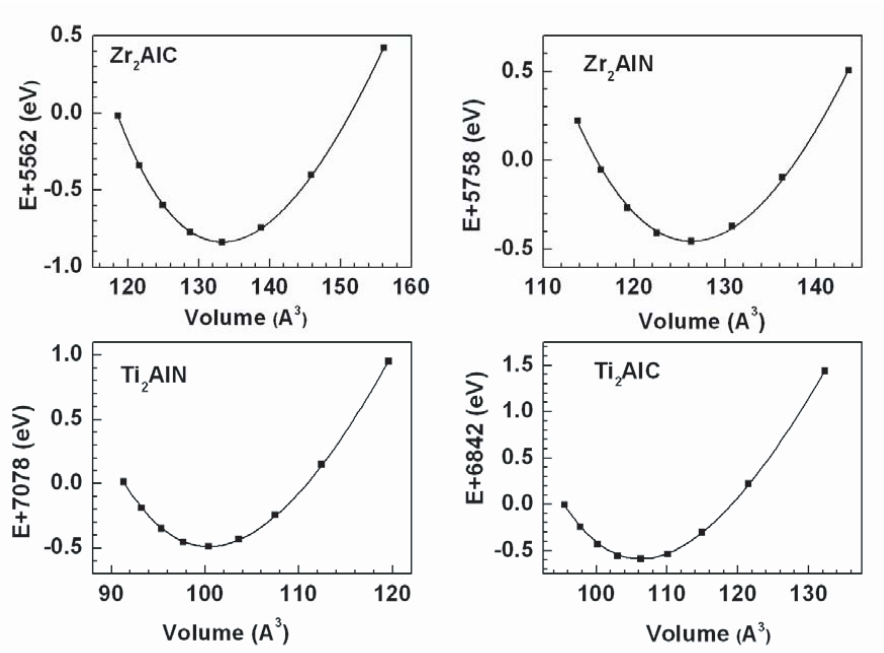


Fig. 3. The calculated pressure-volume relations for Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN . The solid lines are given by the Birch-Murnaghan equation of state with the parameters listed in Table 1.

Table 3. The calculated elastic constants, C_{ij} (in GPa), and the shear anisotropic factor, A , for Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN .

| Compound | C_{11} | C_{12} | C_{13} | C_{33} | C_{44} | C_{66} | A |
|-------------|----------|----------|----------|----------|----------|----------|-------|
| Zr_2AlC | 278 | 64 | 67 | 235 | 97 | 107 | 1.024 |
| Zr_2AlN | 285 | 89 | 92 | 266 | 129 | 96 | 1.406 |
| Ti_2AlC | | | | | | | |
| Present | 307 | 58 | 63 | 284 | 118 | 125 | 1.015 |
| Theory [23] | 321 | 76 | 100 | 318 | 144 | 123 | 1.31 |
| Ti_2AlN | 311 | 71 | 102 | 298 | 133 | 120 | 1.313 |

merely note that the width of the bounds on the shear modulus is related to the anisotropy constant

$$A = 4C_{44}/(C_{11} + C_{33} - 2C_{13}). \quad (2)$$

As A approaches unity the crystal becomes isotropic, and the gap between the bounds vanishes. We also calculated the Young's modulus, E , and Poisson's ratio which are frequently measured for polycrystalline materials when investigating their hardness. These quantities are related to the bulk modulus B and the shear modulus G by the following equations [46]

$$E = 9BG/(3B + G) \quad (3)$$

$$\nu = (3B - E)/(6B). \quad (4)$$

The calculated shear anisotropic factors of Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN are given in Table 3. For an isotropic crystal, A is equal to 1, while any value smaller or larger than 1 indicates anisotropy. The magnitude of the deviation from 1 is a measure of the degree of elastic anisotropy of the crystal. The deviation from 1 is larger

for Zr_2AlN (Ti_2AlN) compared to Zr_2AlC (Ti_2AlC). This conclusion is in agreement with hydrostatic pressure effect results. The calculated bulk and shear moduli for Ti_2AlC are in good agreement with the measured ones.

In the following paragraph we study the pressure dependence of the elastic properties. In Figure 4, we present the variation of the elastic constants ($C_{11}, C_{12}, C_{13}, C_{33}, C_{44}$) and the bulk modulus B of Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN with respect to the variation of pressure. We observe a linear dependence in all curves of these compounds in the considered range of pressure. In Table 5, we listed the results of the pressure derivatives $\partial C_{11}/\partial P$, $\partial C_{12}/\partial P$, $\partial C_{13}/\partial P$, $\partial C_{33}/\partial P$, $\partial C_{44}/\partial P$ and $\partial B/\partial P$ for the four considered compounds. It is easy to observe that the elastic constants C_{ij} and bulk modulus B increase when the pressure is enhanced in these four compounds. To our knowledge no experimental or theoretical data for the pressure derivative of elastic constants of Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN are mentioned in the literature. Then, our results can provide reference data for future investigations.

3.3 Calculation of Debye temperature

We estimated the Debye temperature (θ_D) of Zr_2AlC and Zr_2AlN from the averaged sound velocity, ν_m , using the following equation [23, 48]:

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

where h is Planck's constant, k_B Boltzmann's constant and V_a the atomic volume. The average sound velocity in the

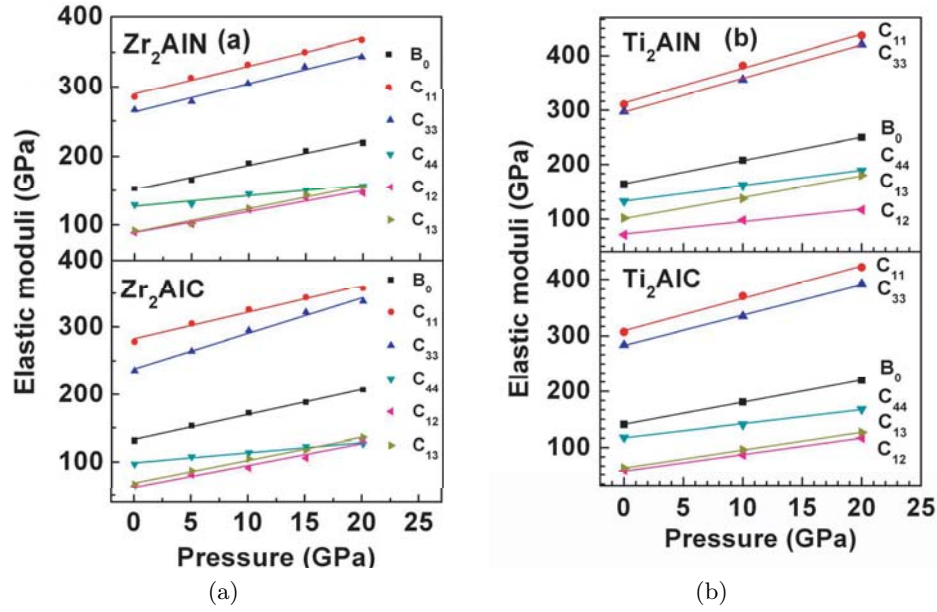


Fig. 4. The calculated pressure dependence of the elastic constants (C_{11} , C_{12} , C_{13} , C_{33} and C_{44}) and the bulk modulus (B) for Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN compounds.

Table 4. The calculated shear moduli (in GPa), G_R , G_V , and $G = (G_R + G_V)/2$, bulk moduli (in GPa), B_V , B_R , and $B = (B_R + B_V)/2$ and Young's modulus (in GPa), E , for Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN , along with the available experimental and theoretical data.

| Compound | B_R | B_V | B | G_R | G_V | G | E | ν |
|-------------|-------|-------|-------|-------|-------|-------|-------|--------|
| Zr_2AlC | 131.2 | 131.9 | 131.6 | 99.2 | 99.7 | 99.5 | 238.4 | 0.1981 |
| Zr_2AlN | 153.4 | 153.6 | 153.5 | 106.2 | 108.7 | 107.0 | 260.6 | 0.2171 |
| Ti_2AlC | | | | | | | | |
| Present | 140.6 | 140.7 | 141 | 119.2 | 119.3 | 119 | 279 | 0.1686 |
| Expt. [10] | | | 144 | | | 118 | 227 | 0.19 |
| Theory [23] | 163.9 | 168.0 | 166 | 127.4 | 127.8 | 127.6 | | |
| Ti_2AlN | 163.2 | 163.3 | 163 | 118.3 | 108.7 | 114 | 276 | 0.2177 |

polycrystalline material is given by [23, 48]:

$$\nu_m = \left[\frac{1}{3} \left(\frac{2}{\nu_t^3} + \frac{1}{\nu_l^3} \right) \right]^{-1/3} \quad (6)$$

where ν_l and ν_t are the longitudinal and transverse sound velocity obtained using the shear modulus G and the bulk modulus B from Navier's equation [23, 46]:

$$\nu_l = \left(\frac{3B + 4G}{3\rho} \right)^{1/2} \quad \text{and} \quad \nu_t = \left(\frac{G}{\rho} \right)^{1/2}. \quad (7)$$

The calculated sound velocity and Debye temperature as well as the density for Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN are given in Table 6. Unfortunately, as far as we know, there are no data available related to these properties in the literature for Zr_2AlC and Zr_2AlN . Future experimental work will testify our calculated results. For Ti_2AlC and Ti_2AlN , the calculated Debye temperatures are in good agreement with the experimental ones. This

Table 5. The calculated pressure derivatives of the elastic moduli for Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN compounds.

| Compound | $\frac{\partial B}{\partial P}$ | $\frac{\partial C_{11}}{\partial P}$ | $\frac{\partial C_{33}}{\partial P}$ | $\frac{\partial C_{44}}{\partial P}$ | $\frac{\partial C_{12}}{\partial P}$ | $\frac{\partial C_{13}}{\partial P}$ |
|-----------|---------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|
| Zr_2AlC | 3.74 | 3.98 | 5.28 | 1.5 | 3.26 | 3.38 |
| Zr_2AlN | 3.48 | 4.02 | 4.10 | 1.54 | 3.04 | 3.36 |
| Ti_2AlC | 3.95 | 5.75 | 5.4 | 2.5 | 2.95 | 3.2 |
| Ti_2AlN | 4.3 | 6.4 | 6.1 | 2.8 | 2.3 | 3.9 |

Table 6. The calculated density (ρ in g/cm^3), the longitudinal, transverse and average sound velocity (ν_l , ν_t , ν_m in m/s) calculated from polycrystalline elastic modulus, and the Debye temperatures (θ_D in K) calculated from the average sound velocity for Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN compounds, along with the available experimental and theoretical data.

| Compound | ρ | ν_l | ν_t | ν_m | θ_D |
|-------------|--------|---------|---------|---------|------------|
| Zr_2AlC | 5.56 | 6891 | 4228 | 4667 | 544 |
| Zr_2AlN | 5.88 | 7000 | 4268 | 4720 | 561 |
| Ti_2AlC | | | | | |
| Present | 4.25 | 8400 | 5303 | 5836 | 733 |
| Expt. [10] | 4.1 | 8525 | 5298 | | 732 |
| Expt. [12] | | | | | 672 |
| Theory [23] | 4.03 | 9133 | 5627 | 6209 | 770 |
| Ti_2AlN | | | | | |
| Present | 4.496 | 8365 | 5025 | 5558 | 711 |
| Expt. [12] | | | | | 679 |

good agreement between calculated and experimental Debye temperatures is gratifying and support that our calculations are reliable and accurate.

4 Conclusions

Employing PP-PW approach based on density functional theory, within the local density approximation, we studied the structural and elastic properties of Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN compounds under pressure effect. A summary of our results follows.

- (i) The calculated structural parameters at zero-pressure are in agreement with the available data.
- (ii) The pressure dependence of the relative lattice parameters (a/a_0 , c/c_0 , c/a) and internal structural parameter (z) fit a quadratic relation.
- (iii) A numerical first-principles calculation of the elastic constants was used to calculate C_{11} , C_{12} , C_{13} , C_{33} , C_{44} and C_{66} . We found a linear dependence of the bulk modulus and elastic constants versus applied pressure.
- (iv) We calculated the shear modulus G , Young's modulus E , and Poisson's ratio ν , for ideal polycrystalline Zr_2AlX and Ti_2AlX aggregates.
- (v) We derived the sound velocity and the Debye temperature for Zr_2AlC , Zr_2AlN , Ti_2AlC and Ti_2AlN compounds.

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