

# First-principles study of structural and elastic properties of $\text{Sc}_2\text{AC}$ ( $A = \text{Al}, \text{Ga}, \text{In}, \text{Tl}$ )

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## Abstract

Using first-principles calculations, the structural and elastic properties of  $\text{Sc}_2\text{AC}$ , with  $A = \text{Al}, \text{Ga}, \text{In}$  and  $\text{Tl}$ , 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 effect of high pressures, up to 20 GPa, on the lattice constants and the internal parameters is calculated. The elastic constants 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  $\text{Sc}_2\text{AC}$  aggregates. We estimated the Debye temperature of  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TlC}$  compounds, and it still awaits the experimental confirmation.

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## 1. Introduction

$\text{M}_2\text{AX}$  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 associated metals and ceramics (for details see Ref. [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 60  $\text{M}_2\text{AX}$  phases have been discovered, among them there are some  $\text{Sc}_2\text{AX}$  phases.

The  $\text{M}_2\text{AlX}$  phases with  $M = (\text{Ti}, \text{V}, \text{Cr}, \text{Nb}, \text{Ta}, \text{Zr}, \text{Hf})$  and  $X = (\text{N}, \text{C})$  have been experimentally and

theoretically extensively studied [1–29]. However, there are few studies on  $\text{Sc}_2\text{AC}$  [30]. The elastic constants are among the properties which are not yet calculated or measured for  $\text{Sc}_2\text{AC}$  compounds. Moreover, it seems that there are no studies about the strain effect on the structural properties of  $\text{Sc}_2\text{AC}$  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 the calculations or measurements has become quite interesting in the recent few years as it provides insight into the nature of the solid-state theories and determines the values of fundamental parameters [31].

We therefore think that it is worthwhile to perform calculations for the structural and elastic properties of  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TlC}$  using the ultra-soft pseudo-

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Table 1  
Structural parameters of Sc<sub>2</sub>AlC, Sc<sub>2</sub>GaC, Sc<sub>2</sub>InC and Sc<sub>2</sub>TlC 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 available calculated results

Compound		$a_0$ (Å)	$c_0$ (Å)	$c_0/a_0$	$B_0$ (GPa)	$B'$	$z$
Sc <sub>2</sub> AlC	Present	3.2275	14.8729	4.6081	95	3.55	0.0824
	Ref. [30]	3.28	15.3734	4.687	99		
Sc <sub>2</sub> GaC	Present	3.2363	14.3949	4.448	97	3.82	0.0852
	Ref. [30]	3.253	15.8128	4.861	96		
Sc <sub>2</sub> InC	Present	3.2752	15.082	4.605	96	4.13	0.0803
	Ref. [30]	3.272	16.4516	5.028	93		
Sc <sub>2</sub> TlC	Present	3.30	14.9856	4.5410	96	4.3	0.0805
	Ref. [30]	3.281	16.5297	5.038	90		

The values of  $B_0$  and  $B'$  are evaluated from the fitting of the pressure–volume data to an analytical equation of state.

potential plane-waves (PP-PW) method in order to provide reference data for the experimentalists on this fascinating class of materials.

## 2. Computational methods

The first-principles calculations are performed by employing pseudo-potential plane-waves (PP-PW) approach based on the density functional theory (DFT) [32,33] and implemented in the most recent version of CASTEP (Cambridge Serial Total Energy Package) code [34]. The major advantages of this approach are: the ease of computing forces and stresses; good convergence control with respect to all computational parameters employed; favourable scaling with number of atoms in the system and the ability to make cheaper 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 [35,36]. The presence of tightly-bound core electrons was represented by nonlocal ultra-soft pseudo-potentials of the Vanderbilt-type [37]. The states C 2s<sup>2</sup>2p<sup>2</sup>, Sc 3s<sup>2</sup>3p<sup>2</sup>3d<sup>1</sup>4s<sup>2</sup>, Al 4d<sup>10</sup>5s<sup>2</sup>5p<sup>1</sup>, Ga 3d<sup>10</sup>4s<sup>2</sup>4p<sup>1</sup>, In 4d<sup>10</sup>5s<sup>2</sup>5p<sup>1</sup> and Tl 4d<sup>10</sup>5s<sup>2</sup>5p<sup>1</sup> were treated as valence states. 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 × 9 × 2 special k-points mesh [38]. The size of the basis set is given by cut-off energy equal to 350 eV. Careful convergence tests show that with these parameters relative energy converged to better than 5 × 10<sup>−6</sup> eV/atom.

## 3. Results and discussion

### 3.1. Structural properties

Sc<sub>2</sub>AC (A = Al, Ga, In, Tl) compounds crystallize in the Cr<sub>2</sub>AlCd crystal structure, with space group *P*6<sub>3</sub>/*mmc* (#194). Its unit cell contains two molecules. The C atoms are positioned at the (0, 0, 0) positions, the A atoms at (1/3, 2/3, 3/4) and the four Sc atoms at (1/3, 2/3,  $z$ ) [26]. The structure is thus defined by two lattice parameters,  $a$  and  $c$ , and the internal structural parameter,  $z$ .

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 Å<sup>−1</sup> and the cell parameters were relaxed until total stresses were below 0.02 eV Å<sup>−3</sup>. The calculated lattice parameters,  $a_0$  and  $c_0$ , and the internal structural parameter  $z$ , for Sc<sub>2</sub>AC (A = Al, Ga, In, Tl) as determined from geometry at  $P = 0$  GPa, are given in Table 1 together with the available theoretical data. There is a reasonable agreement between our results and those calculated by Music et al. [30]. The slight underestimation of the lattice constants compared to those of Ref. [30] is due to the use of the LDA which is known to underestimate the lattice constants compared to the measured ones. Note that the GGA used by Ref. [30] is known to overestimate the lattice constants compared to measurements.

In order to show how the structural parameters under pressure in these compounds behave, the equilibrium geometries of Sc<sub>2</sub>AlC, Sc<sub>2</sub>GaC, Sc<sub>2</sub>InC and Sc<sub>2</sub>TlC 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 there were no phase transformations observed in Ti<sub>2</sub>AlN, Ti<sub>2</sub>AlC, V<sub>2</sub>AlC, Cr<sub>2</sub>AlC, Nb<sub>2</sub>AlC, Nb<sub>2</sub>TiC and Zr<sub>2</sub>InC samples up to pressures ≈50 GPa by using a synchrotron radiation and a diamond–anvil cell to measure the pressure dependencies of the lattice parameters of these compounds [11,25,39]. Figs. 1 and 2 plot the variation of the relative changes of the lattice parameters ( $a/a_0$  and  $c/c_0$ ) and the internal parameter ( $z$ ) versus applied hydrostatic pressure ( $p$ ), respectively. The pressure lattice parameters data have been fitted with a quadratic polynomial. The same behaviour has been observed previously for Ti<sub>2</sub>AlN and Ti<sub>2</sub>AlC [11], M<sub>2</sub>AlC (M = Ti, V, Cr, Nb, and Ta) [25], Ti<sub>3</sub>Si<sub>0.5</sub>Ge<sub>0.5</sub>C<sub>2</sub> [40], Ti<sub>3</sub>GeC<sub>2</sub> [41], Ti<sub>4</sub>AlN<sub>3</sub> [42], Ti<sub>2</sub>SC [43], Zr<sub>2</sub>InC [39] and M<sub>2</sub>GaC (M = Ti, V, Nb and Ta) [44]. The solid curve is the quadratic least-squares fit. The values of the linear and quadratic pressure coefficients of  $a/a_0$ ,  $c/c_0$  and  $z$  for these compounds are given in Table 2.

The calculated unit cell volumes at fixed values of applied hydrostatic pressure in the range from 0 to 20 GPa with the

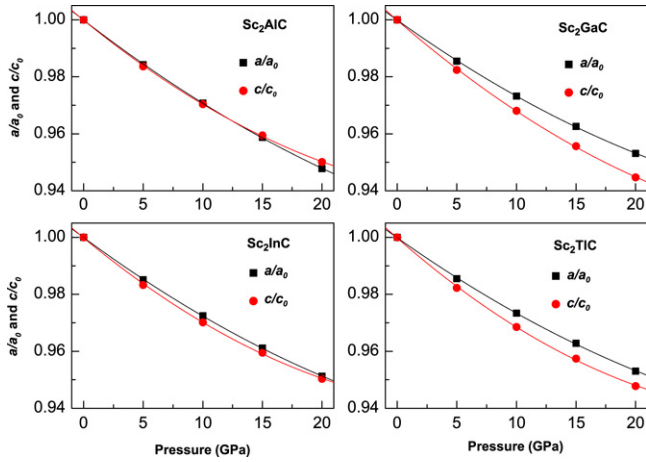


Fig. 1. Pressure dependence of the relative lattice parameters ( $a/a_0$  and  $c/c_0$ ) for  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TiC}$  compounds. The solid lines are least-square fits of the data points to a quadratic polynomial.

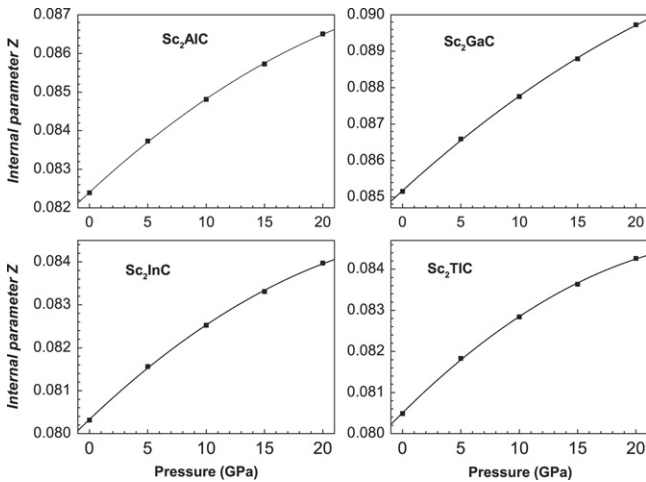


Fig. 2. Pressure dependence of the internal structural parameter ( $z$ ) for  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TiC}$  compounds. The solid lines are least-square fits of the data points to a quadratic polynomial.

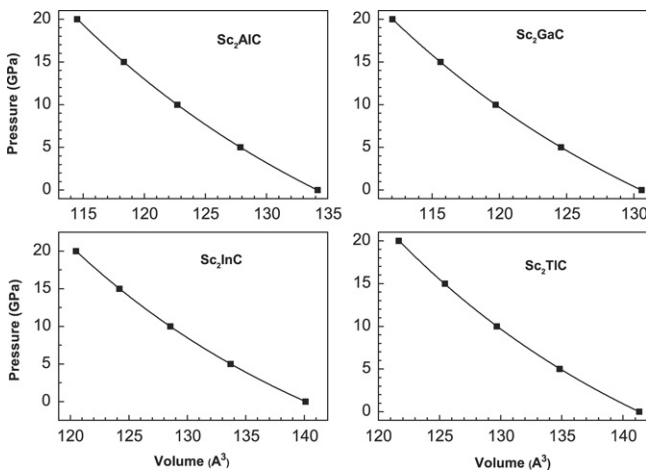


Fig. 3. The calculated pressure–volume relations for  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TiC}$  compounds. The solid lines are given by the Birch–Murnaghan equation of state with the parameters listed in Table 1.

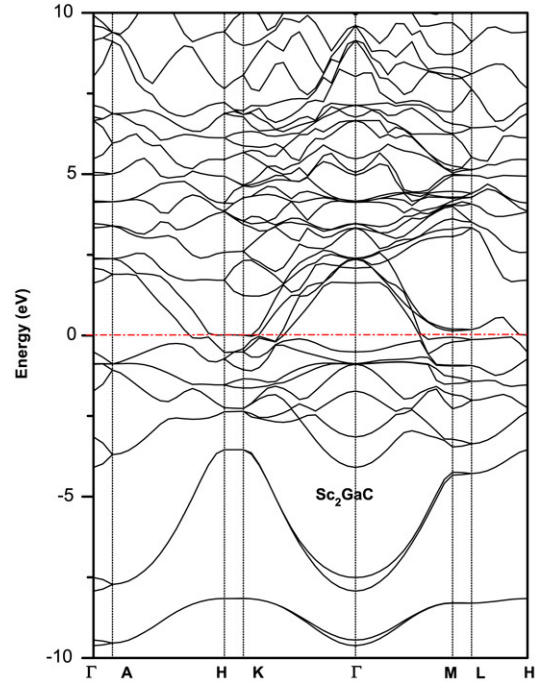


Fig. 4. Band structures along the principal high-symmetry directions in the Brillouin zone of  $\text{Sc}_2\text{GaC}$ .

step of 5 GPa were used to construct the equation of state (EOS), which was fitted to a third-order Birch–Murnaghan equation [45] (Fig. 3)

$$P = \frac{3}{2}B_0 \left[ \left( \frac{V_0}{V} \right)^{\frac{7}{3}} - \left( \frac{V_0}{V} \right)^{\frac{5}{3}} \right] \left[ 1 + \frac{3}{4}(4 - B') \times \left\{ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right\} \right] \quad (1)$$

with  $V_0$  fixed at the value determined from the zero-pressure data. We obtained, by least-squares fitting, the bulk modulus  $B_0$  and its pressure derivative  $B'$  at zero pressure. These are listed in Table 1.

### 3.2. Electronic properties

The calculated energy band structure, at equilibrium lattice parameters for  $\text{Sc}_2\text{GaC}$ , along the high-symmetry directions in the Brillouin zone is shown in Fig. 4 as a prototype since the band profiles are quite similar (with slight differences) for all the four compounds. The valence and conduction bands overlap considerably and there is no band gap at the Fermi level. This finding indicates the metallicity of these four materials.

The calculated total densities of states (DOS) for  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TiC}$  are shown in Fig. 5. The overall DOS spectrum profiles are in fairly good agreement with the previous theoretical results [30]. There is no band gap for the four materials and the DOS has a large finite value at the Fermi level. Once again, this finding confirms the metallicity of these materials.

Table 2  
The calculated first- ( $\alpha$  in  $10^{-4}$  GPa $^{-1}$ ) and second-order ( $\beta$  in  $10^{-5}$  GPa $^{-2}$ ) pressure coefficients of the relative lattice parameters ( $a/a_0$ ,  $c/c_0$ ) and internal structural parameter ( $z$ ) for Sc<sub>2</sub>AlC, Sc<sub>2</sub>GaC, Sc<sub>2</sub>InC and Sc<sub>2</sub>TiC

	Sc <sub>2</sub> AlC		Sc <sub>2</sub> GaC		Sc <sub>2</sub> InC		Sc <sub>2</sub> TiC	
	$\alpha$	$\beta$	$\alpha$	$\beta$	$\alpha$	$\beta$	$\alpha$	$\beta$
$a/a_0$	-32.30	3.1554	-30.00	3.3105	-30.8	3.2594	-29.6	3.1370
$c/c_0$	-34.10	4.6639	-36.20	4.3731	-34.6	4.9967	-36.6	5.3912
$z$	2.786	-0.3711	2.9103	-0.3211	2.5846	-0.3863	2.8099	-0.4694

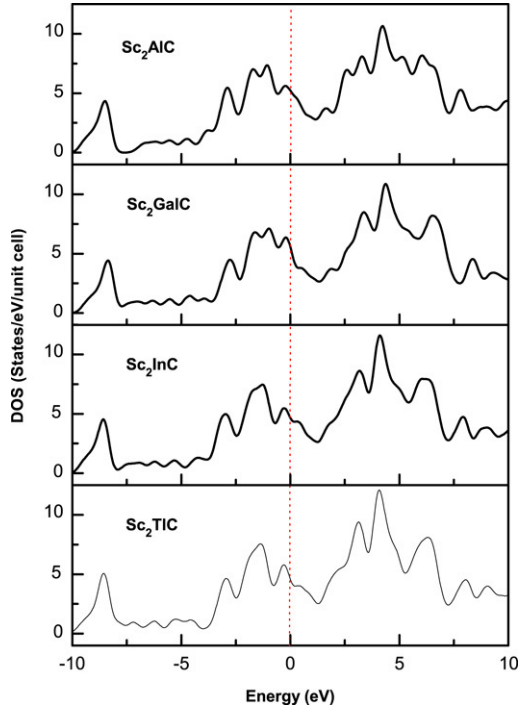


Fig. 5. Total density of states for Sc<sub>2</sub>AlC, Sc<sub>2</sub>GaC, Sc<sub>2</sub>InC and Sc<sub>2</sub>TiC compounds.

### 3.3. Elastic properties

It is well established that first-principle studies based on DFT can be used to obtain reliable elastic properties of inorganic compounds [46,47]. 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  $\overset{\leftrightarrow}{C}$  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 becomes  $\sigma_i = C_{ij} \varepsilon_j$ . 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  $6 \times 6$  symmetric matrix with a maximum of 21 different components, such that  $\sigma_i = C_{ij} \varepsilon_j$  for small stresses  $\sigma$ , and strains,  $\varepsilon$  [48,49]. Any symmetry present in the structure may make some of these components equal and may let 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 nonzero first and fourth components, and another with a nonzero third component, give stresses related to all five independent elastic coefficients for the hexagonal system [50–52]. 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.

In Table 3, we listed the calculated values of the elastic constants  $C_{ij}$ . The errors quoted for  $C_{ij}$ -values are associated with the deviation of the stress–strain relationship from linearity. 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 [53]. 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, the Reuss bulk modulus ( $B_R$ ) and the Reuss shear modulus ( $G_R$ ), for all lattices [53,54], while Voigt discovered upper bounds, the Voigt bulk modulus ( $B_V$ ) and the Voigt shear modulus ( $G_V$ ) [53,55]. Hill has shown that the Voigt and Reuss averages are limits and suggested that the actual effective moduli could be approximated by the arithmetic mean of the two bounds [56]. 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 [53]:

$$E = 9BG/(3B+G) \quad (2)$$

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

The calculated bulk modulus  $B$ , shear modulus  $G$ , Young's modulus  $E$ , and Poisson's ratio of Sc<sub>2</sub>AlC, Sc<sub>2</sub>GaC, Sc<sub>2</sub>InC

Table 3

The calculated elastic constants,  $C_{ij}$  (in GPa) for  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TlC}$ ; the errors are obtained from the statistical analysis

Compound	$C_{11}$	$C_{33}$	$C_{44}$	$C_{12}$	$C_{13}$	$C_{66}$
$\text{Sc}_2\text{AlC}$	$186 \pm 1.5$	$189 \pm 1.5$	$48 \pm 0.5$	$58 \pm 0.7$	$40 \pm 0.6$	$64 \pm 1$
$\text{Sc}_2\text{GaC}$	$177 \pm 2$	$181 \pm 1$	$45 \pm 1$	$77 \pm 1$	$44 \pm 0.5$	$50 \pm 1$
$\text{Sc}_2\text{InC}$	$206 \pm 2$	$191 \pm 2$	$50 \pm 3$	$51 \pm 1$	$38 \pm 0.5$	$77 \pm 1$
$\text{Sc}_2\text{TlC}$	$199 \pm 1$	$172 \pm 3$	$50 \pm 3$	$52 \pm 1$	$35 \pm 1$	$73 \pm 1$

Table 4

The calculated bulk moduli (in GPa),  $B_V$ ,  $B_R$ , and  $B_0 = (B_R + B_V)/2$ , shear moduli (in GPa),  $G_R$ ,  $G_V$ , and  $G = (G_R + G_V)/2$ , Young's modulus (in GPa),  $E$ , and Poisson's ratio,  $\nu$ , for  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TlC}$

Compound	$B_R$	$B_V$	$B_0$	$G_R$	$G_V$	G	E	$\nu$
$\text{Sc}_2\text{AlC}$	93	93	93	58.2	60.2	59.2	146	0.23732
$\text{Sc}_2\text{GaC}$	95.7	96.1	96	50.9	52.7	51.8	132	0.27111
$\text{Sc}_2\text{InC}$	94.9	95.2	95	64	67.2	65.6	160	0.21945
$\text{Sc}_2\text{TlC}$	89.5	90.4	90	62.1	64.6	63.3	154	0.21496

and  $\text{Sc}_2\text{TlC}$  are given in Table 4. From Tables 1 and 4, we can see that the calculated value of the bulk modulus ( $B$ ) from the elastic constants (Table 4) has nearly the same value as the one obtained from the EOS fitting ( $B_0$ ) (Table 1). This might be an estimate of the reliability and accuracy of our calculated elastic constants for the  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TlC}$  compounds.

### 3.4. Calculation of Debye temperature

We estimated the Debye temperature ( $\theta_D$ ) of  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TlC}$  from the averaged sound velocity,  $v_m$ , using the following equation [23,57]:

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

where  $h$  is Planck's constant,  $k_B$  Boltzmann's constant and  $V_a$  the atomic volume. The average sound velocity in the polycrystalline material is given by [23,57]:

$$v_m = \left[ \frac{1}{3} \left( \frac{2}{v_l^3} + \frac{1}{v_t^3} \right) \right]^{-1/3} \quad (5)$$

where  $v_l$  and  $v_t$  are the longitudinal and transverse sound velocity obtained using the shear modulus  $G$  and the bulk modulus  $B$  from Navier's equation [23,58]:

$$v_l = \left( \frac{3B + 4G}{3\rho} \right)^{1/2} \quad \text{and} \quad v_t = \left( \frac{G}{\rho} \right)^{1/2}. \quad (6)$$

The calculated sound velocity and Debye temperature as well as the density for  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TlC}$  are given in Table 5. Unfortunately, as far as we know, there are no data available related to these properties in the literature for these compounds. Future experimental work will testify our calculated results.

## 4. Conclusions

Employing PP-PW approach based on the density functional theory, within the local density approximation, we studied the

Table 5

The calculated density ( $\rho$  in  $\text{g/cm}^3$ ), the longitudinal, transverse and average sound velocity ( $v_l$ ,  $v_t$ ,  $v_m$  in m/s) calculated from polycrystalline elastic modulus, and the Debye temperatures ( $\theta_D$  in K) calculated from the average sound velocity for  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TlC}$  compounds, along with the available experimental data

Compound	$\rho$	$v_l$	$v_t$	$v_m$	$\theta_D$
$\text{Sc}_2\text{AlC}$	3.19	7340	4308	4775	556
$\text{Sc}_2\text{GaC}$	4.36	6147	3455	3834	450
$\text{Sc}_2\text{InC}$	5.14	5960	3573	3953	453
$\text{Sc}_2\text{TlC}$	7.2	4923	2966	3280	375

structural and elastic properties of  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TlC}$  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 ( $a/a_0$ ,  $c/c_0$ ) and internal structural parameter ( $z$ ) have been fitted with 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  $C_{66}$ .
- (iv) We calculated the shear modulus  $G$ , Young's modulus  $E$ , and Poisson's ratio  $\nu$ , for ideal polycrystalline  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TlC}$  aggregates.
- (v) We derived the sound velocity and the Debye temperature for  $\text{Sc}_2\text{AlC}$ ,  $\text{Sc}_2\text{GaC}$ ,  $\text{Sc}_2\text{InC}$  and  $\text{Sc}_2\text{TlC}$  compounds.

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