# Mechanical and Elastic Properties of Selected 211 MAX Phases: A Density Functional Theory Study

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## ABSTRACT

MAX Phases are a class of ternary materials that have continued to play a greater role in the field of materials science due to their unique properties that bridge the gap between metals and ceramics which have uses in a wide range of applications. However, in spite of these progress, there are still a lot of open questions and properties that needs to be understood. The Mechanical and elastic properties of (Nine) MAX phase materials, namely, $Ti_2AlC$, $Ti_2AlN$, $Ti_2GaC$, $Ti_2GaN$, $Ti_2PbC$, $Ti_2CdC$, $Ti_2SiC$, $Ti_2GeC$ and $Ti_2SnC$ have been investigated using the density functional theory within the generalized gradient approximations as expressed in Quantum Espresso and VASP codes. The values of elastic anisotropy, Young's modulus, Poisson ratio and shear modulus revealed that the compounds were indeed stable and ductile. Out of all the nine MAX Phase materials, $Ti_2PbC$ and $Ti_2CdC$ are more stable than the other considered compounds. The findings of this study suggest that the nine MAX phases are potential candidates in various industrial applications requiring hard materials.

**Keywords:** Elastic constants, MAX phases, Mechanical properties

## I. INTRODUCTION

MAX phases are ternary materials that have gained prominence in 1990's when these ternary carbide and nitride materials were found to bridge the gap between metals and ceramics. The materials pose a general formula $M_{n+1}AX_n$, where M is an early transition metal, A represents an A group element, X represents C and/or N, and n=1 to 3. These compounds are also known as metallic ceramics (Ghosh & Harimkar, 2012). Based on the value of n, different MAX phase materials can be obtained. For example, when n=1,2 and 3, $M_2AX$, $M_3AX_2$ and $M_4AX_3$ phases are obtained and these are usually referred to as 211, 312 and 413 phases respectively. With the availability of more computing power and advanced experiments, higher order MAX phases such as 514, 615 and 716 (Sun, 2011) have also been predicted.

MAX phase materials combine the properties of each of the three elements, to result into a final compound that has applications in a wide range of fields. These include areas like transportation, industrial application, kiln furnace, heat exchangers, exhaust gas filters for automobiles, free-cutting elements, microelectronics and biomaterials, damping materials, corrosion resistant materials and surface coatings, substrates for CVD (chemical vapour deposition) diamond among others (Berger, 2020). MAX_phase compounds are also being investigated for catalysis applications (Akshay *et al.*, 2021).

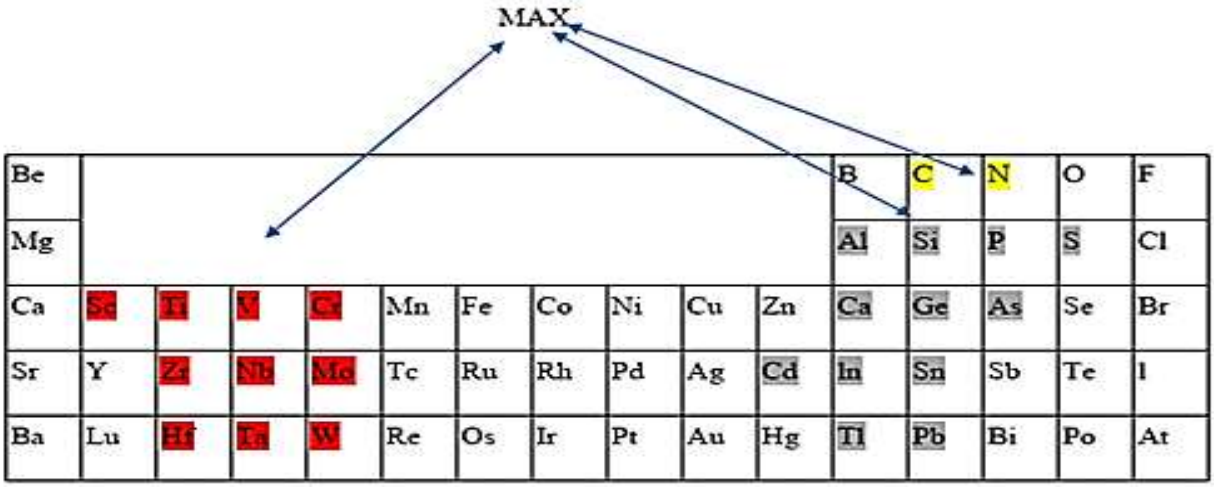
The major contributing factor for the increased research on MAX phases lies on their unique and unusual properties (Barsoum & Radovic, 2011; Nowotny, 1970). This is attributed to their atomic chemical bonding and structural characteristics. These materials are resistant to chemical attack with relatively low thermal expansion coefficients (Radovic, 2013).

In terms of mechanical properties, these materials are relatively soft (Eklund, *et al.*, 2010), readily machinable, thermal shock resistant, and damage tolerant (Ouyang, 2006). Some of these compounds include $Ti_3SiC_2$, $Ti_3GeC_2$, $Ti_3AlC_2$, $Ti_3SnC_2$ and $Ta_3AlC_2$ among others and they are fatigue, creep, and oxidation resistant. They can be compressed to stresses as high as 1GPa at room temperature, and still recover upon removal of the load while dissipating 25% of the mechanical energy. At higher temperatures, they undergo a brittle-to plastic transition (BPT) state, and their mechanical behaviour is a strong function on the rate of deformation (Barsoum & Radovic, 2011). With two formula units per unit cell, MAX phases are layered hexagonal crystal formations with the space group P63/mmc. The octahedral positions between the tightly packed M layers and the pure A-group element layers that make up the unit cells of the MAX phases are filled with X atoms. Barsoum *et al*. (2011) has reported a number of $M_4AX_3$ or 413 phases and the list has grown since that structure was established in $Ti_4AlN_3$. The A elements are mostly group III A and IV A (i.e. groups 13 to 16); the most versatile of these elements being Al because it entirely forms nine compounds including two nitrides, one 312 phase, and four 413 phases. Ga on the other hand forms nine 211 phases, six of which are carbides and three are nitrides. Similar to MX phases, MAX phase bonding is a combination of metallic, covalent and ionic bonds. Generally, the M-X bonds are stronger than M-A bonds (Barsoum & Radovic, 2011; Radovic, 2013) thus preferring carbides and nitrides formation.

Significant amount of research efforts has been made to understand the physical properties of $M_2AX$ phases both theoretically and experimentally (Horlait *et al.*, 2016; Yoo *et al.*, 2000). Currently, there are approximately 155 MAX compositions that have been synthesized (Sokolc *et al.*, 2019). Most of those studied so far have been carried out with Al as an A element and C as *X* element in MAX-series (Dhakal *et al.*, 2015). Cover *et al.* (2008) did a theoretical survey of $M_2AX$ phase materials using density functional theory and the plane wave potential formalism as implemented in the VASP code (Shishkin & Kresse, 2006), while Dhakal *et al.* (2015) studied the temperature dependent lattice thermal conductivity ($\kappa_{ph}$) of 211, 312 and 413 MAX phase compounds using the equation derived by Slack (Morelli & Slack, 2006) together with the published elastic coefficients on MAX phases. They studied a total of five hundred and fifty-one (551) MAX phase compounds (Dhakal *et al.*, 2015), and probably due to the large number, they ended up reporting a scattered range of phonon thermal conductivity values for the many materials. Roknuzzaman *et al.* (2016) predicted the elastic and optical properties of only two $M_2AX$ phase materials, namely $Ti_2CdN$ and $Ti_2CdC$ using the density functional theory as implemented in CASTEP code (Segall *et al.*, 2002). Incidentally, these are too few to represent the general behaviour or trend of the $M_2AX$ series. According to their results, $Ti_2CdN$ appeared to be stiffer than the already synthesized $Ti_2CdC$, which is used in many engineering applications. Qian *et al* (2012), investigated the structural, electronic, mechanical, and optical properties of only one $M_2AX$ material, i.e. the Nano-laminated $M_2PbC$ (M = Ti, Zr and Hf) compounds using first-principles methods based on the DFT as implemented in the CASTEP code (Segall *et al.*, 2002). Their findings revealed that $Ti_2PbC$ had the largest value of shear modulus of 76 GPa among all the MAX phase compounds studied. Several other theoretical investigations (Aryal *et al.*, 2014; Hettinger *et al*, 2004) have already been carried out in studying the mechanical properties of selected $M_2AX$ phase compounds.

**Figure 1:**

*Periodic Table of Elements Forming Nano Laminates of the General Formula Mn+1axn (N= 1, 2, 3, ------) Where M Is a Transitional D Metal, A Is an A Group Elements (Si, Al, S, Sn, etc.) and X Is Carbon or Nitrogen*

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The study objectives in this paper include the structural, mechanical (i.e. bulk modulus, shear modulus, young's modulus, machinability, ductility, poisons ratio as well as stability) as well as the elastic properties ($C_{11}$, $C_{12}$, $C_{13}$, $C_{33}$ and $C_{44}$) of $Ti_2AlC$, $Ti_2AlN$, $Ti_2GaC$, $Ti_2GaN$, $Ti_2PbC$, $Ti_2CdC$, $Ti_2GeC$, $Ti_2SnC$ and $Ti_2SiC$ MAX phases.

## II. METHODOLOGY

The structural and mechanical properties of the MAX phase materials under study were determined using density functional theory (Kohn & Sham, 1965) as implemented in the Quantum Espresso (QE) (Giannozzi *et al.*, 2009; Bouhemadou, 2009; Baroni *et al.*, 2005; Baroni *et al.*, 2011) and VASP (Shishkin & Kresse, 2006) codes. The exchange correlation functional was approximated using the Generalized Gradient Approximation (GGA) as proposed by Perdew, Burke and Ernzerhof (1996). The core electrons were described by the projector augmented wave method (PAW) (Kresse & Joubert, 1999; Blochl, 1994) [in VASP] and ultrasoft pseudopotentials (Kresse & Hafner, 1994) [in QE]. In QE code, plane-wave kinetic energy cut-offs of 60 Ry (for $Ti_2SnC$), 50 Ry (for $Ti_2AlC$, $Ti_2AlN$, $Ti_2GaC$ and $Ti_2GaN$), 40 Ry (for $Ti_2PbC$) and 30 Ry (for $Ti_2CdC$) were used, together with a dense k-point grid of $21\times21\times7$ after a careful convergence scheme. In the case where VASP was used; a kinetic energy cut-off of 520 eV was used to expand the electronic wave functions and the Brillouin zone was sampled using a dense $25\times25\times5$ Monkhorst-Pack k-point grid (Monkhorst and Pack, 1976).

In order to obtain reliable results for the elastic constants, a highly accurate computational method, THERMO-PW method (Sundareswari, *et al*., 2010) and Phonopy code for VASP were employed in this study as implemented in the QE code. This method has previously proved successful in the theoretical prediction of elastic properties of various materials (Sundareswari *et al*., 2010; Born & Huang, 1956). In the case of VASP code, the elastic constants were calculated by the efficient stress-strain method (Page & Saxe, 2002).

## III. RESULTS

### Structural Properties

Table 1 shows lattice parameters for nine MAX phase materials. These parameters are essential in ensuring the optimized structures possessed the expected structures and therefore leading to the expected results in the subsequent calculations. From this table all of them exhibit good agreement when compared to the existing experimental data and other theoretical research, with only a few minor variances being noted.

**Table 1:**

*DFT-GGA Calculated Lattice Parameters a and c [in ˚A] and Hexagonal Ratio c/a Obtained Using VASP and QE Codes, which are Compared with Other Available Experimental and Theoretical Values*

| | *a* | *c* | *c/a* | Remarks |
|---|---|---|---|---|
| $Ti_2AlN$ | 2.98-3.07 | 13.51-13.65 | 4.44-4.55 | This study |
| | 2.96 | 13.65 | 4.61 | Expt. (Bouhemadou, 2009), |
| | 2.99 | 13.63 | - | VASP (Cover *et al.*, 2008) |
| | 2.98 | 13.68 | 4.59 | Expt. (Vincent *et al.*, 1998), |

| | | | | |
|---|---|---|---|---|
| | 3.01 | 13.70 | 4.55 | VASP (Vincent *et al.*,1998), |
| $Ti_2AlC$ | 3.07-3.10 | 13.70-13.82 | 4.46-4.47 | This study |
| | 3.05 | 13.64 | 4.47 | Expt. (Sun, 2011) |
| | 3.04 | 13.60 | 4.34 | Expt. (Magnuson et al., 2017) |
| | 3.07 | 13.73 | - | VASP (Cover *et al.*, 2008), |
| | 3.08 | 13.77 | 4.47 | VASP (Vincent *et al.*,1998) |
| $Ti_2GaC$ | 3.07 | 13.45-13.51 | 4.38-4.40 | This study |
| | 3.07 | 13.52 | 4.40 | Expt. (Atikur et al., 2015) |
| | 3.07 | 13.43 | | CASTEP (Liu *et al.*, 2009), |
| | 3.07 | 13.52 | 4.38 | Expt. (Magnuson et al., 2017) |
| $Ti_2GaN$ | 3.01-3.07 | 13.32-13.51 | 4.38-4.44 | This study |
| | 3.00 | 13.30 | 4.42 | (Barsoum & El-Raghy, 1996), |
| | 2.96 | 13.02 | 4.40 | LDA [VASP] (Bouhemadou, 2009), |
| | 3.02 | 13.32 | 4.41 | GGA [VASP] (Bouhemadou, 2009), |
| $Ti_2SnC$ | 3.17-3.18 | 13.73-13.97 | 4.33-4.39 | This study |
| | 3.16 | 13.68 | 4.33 | Expt. (Vincent *et al.*, 1998), |
| | 3.16 | 13.68 | 4.32 | Expt. (Barsoum *et al.*, 1997), |
| | 3.19 | 13.63 | 4.28 | Expt. (Jeitschko *et al.*, 1963), |
| | 3.17 | 13.86 | 4.37 | PP-PW (Hug, 2006) |
| | 3.16 | 13.64 | 4.35 | ABINIT (Bouhemadou, 2008), |
| | 3.13 | 13.55 | 4.33 | CASTEP (Zhai *et al.*, 2007) |
| | 3.10 | 13.40 | 4.39 | CASTEP (Bouhemadou, 2008) |
| $Ti_2CdC$ | 3.07-3.10 | 14.12-14.45 | 4.66 | This study |
| | 3.10 | 14.41 | 4.65 | Expt. (Jeitschko *et al.*, 1964) |
| | 3.09 | 14.53 | 4.70 | CASTEP (Liu *et al.*, 2009) |
| | 3.10 | 14.55 | 4.69 | CASTEP (Bai *et al.*, 2010) |
| | 3.10 | 14.57 | 4.70 | CASTEP (Born and Huang, 1956) |
| | 3.11 | 14.54 | 4.68 | VASP (Cover *et al.*, 2009) |
| $Ti_2PbC$ | 3.22-3.23 | 13.78-13.99 | 4.28-4.34 | This study |
| | 3.20 | 13.81 | 4.32 | (Sun, 2011) |
| | 3.22 | 13.99 | 4.34 | CASTEP (Liu *et al.*, 2009), |
| | 3.23 | 13.98 | 4.32 | CASTEP (Birch, 1947) |
| | 3.23 | 14.01 | 4.33 | VASP (Cover *et al.*, 2009) |
| $Ti_2SiC$ | 3.05-3.23 | 12.88-13.24 | 4.10-4.22 | This study |
| $Ti_2GeC$ | 3.07-3.09 | 13.50-13.51 | 3.37-3.40 | This study |

Figure 2 shows bond lengths of the nine 211 MAX Phases materials. It was noted that, where available, computed bond lengths were in strong agreement with the corresponding experimental measurements. It is observed that strong bond exist between Ti-X as compared to other bonds because of its shorter bond length.

**Figure 2:**

*Bond Lengths of the Nine 211 MAX Phases Materials*

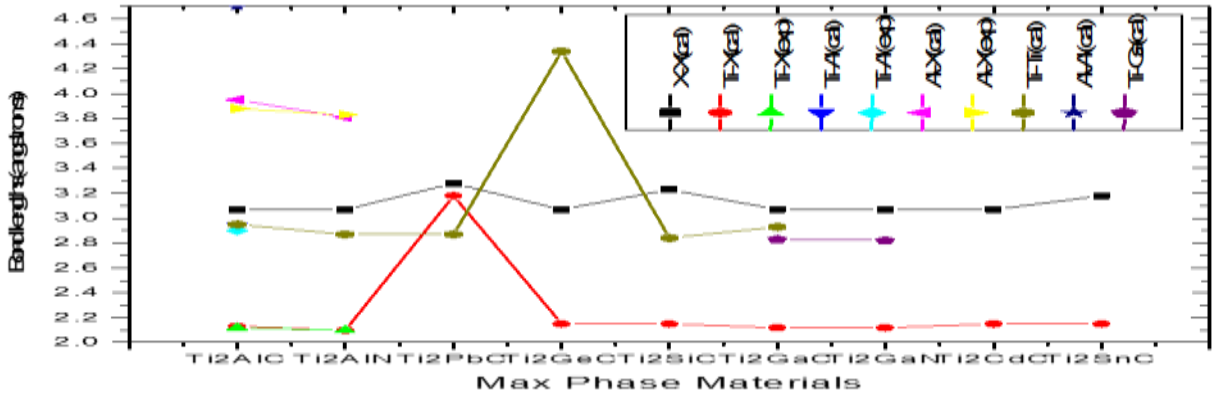
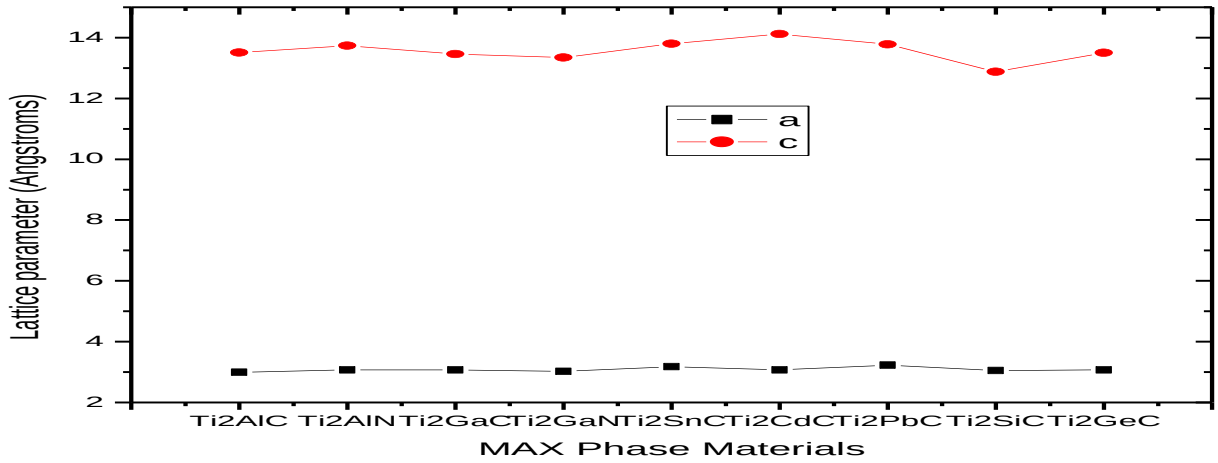



Figure 3 Shows the lattice parameters ***a*** and ***c*** for the $Ti_2AX$ MAX phase materials studied in this paper. The value of ***a*** lies averagely at three (3) Angstroms while the ***c*** lies between 13-14Angstroms for all the materials considered in this study.

**Figure 3:**

*Lattice Parameter (Angstroms) of the Nine Ti2AX MAX Phase Compounds*




## Elastic and Mechanical Properties

This sub-section deals with the elastic and mechanical properties for the nine MAX phase materials considered in this investigation. The results obtained using QE and VASP Codes were compared with other results obtained from different approaches as seen in Table 2 and Table 4. It was discovered that the elastic constants for the investigated hexagonal structures were in good agreement with both experimental results and other theoretical research carried out using various methodologies.

**Table 2:**

*Calculated Elastic Constants Cij (Gpa) for Ti2AlC, Ti2AlN, Ti2GaC, Ti2GaN, Ti2PbC, Ti2CdC, Ti2SnC, Ti2SiC and Ti2GeC MAX Phases Obtained Using VASP and QE Codes Compared with Available Reported Data*

| | *C*11 | *C*12 | *C*13 | *C*33 | *C*44 | Reference |
|---|---|---|---|---|---|---|
| $Ti_2AlN$ | 272.1* , 308.4# | 56.8 *,75.3# | 86.9* ,89.5 | 271.3*, 287.2# | 121.1* ,118.6# | This Calc. |
| | 342 | 56 | 96 | 283 | 123 | (Rahaman *et al.*, 2015) |
| | 309 | 66 | 91 | 280 | 125 | (Cover, 2008) |
| $Ti_2AlC$ | 274.7*, 297.3# | 50.4*, 63.6# | 49.3 *, 59# | 246.8 *, 262# | 101.7 *, 110# | This Calc. |
| | 301 | 59 | 55 | 278 | 113 | (Rahaman *et al.*, 2015) |
| | 302 | 62 | 61 | 269 | 109 | (Cover, 2008) |
| $Ti_2GaC$ | 275.9*, 306.4# | 59.5* , 65.6# | 46.5*, 60.6# | 225.5*, 265.9# | 89.8*, 114# | This Calc. |
| | 314 | 66 | 59 | 272 | 122 | (Rahaman *et al.*, 2015) |
| $Ti_2GaN$ | 267.9*, 293# | 70.3*, 89.9# | 85.4*, 91.6# | 249.5*, 272.9# | 107.5*, 113# | This Calc. |
| | 338±2 | 97±2 | 111±0.8 | 312±3 | 136±1 | LDA (Cover, 2008) |
| | 296±1 | 84±0.7 | 92±0.4 | 275±3 | 119±0.5 | GGA (Cover, 2008) |
| $Ti_2SnC$ | 228.0 *, 265.5# | 74.2* , 78.2# | 47.7*, 71.2# | 202.7*, 263# | 74.0*, 91# | This Calc. |
| | 260 | 78 | 70 | 254 | 93 | (Rahaman *et al.*, 2015) |
| $Ti_2CdC$ | 226.5*, 251.1# | 59.2* , 73.2# | 43.8* , 44.9# | 183.6* , 203.6# | 29.8*, 36# | This Calc. |
| | 258 | 68 | 46 | 205 | 33 | (Rahaman *et al.*, 2015) |
| $Ti_2PbC$ | 202.5* , 239.1# | 81.9* , 90.6# | 49.7* , 51.4# | 195.7* , 213.2# | 60.8* , 65.1# | This Calc. |
| | 235 | 90 | 53 | 211 | 66 | (Rahaman *et al.*, 2015) |
| $Ti_2GeC$ | 258.5*, 281.6# | 53.3*, 79.3# | 83.5*, 96# | 260.7*, 286.7# | 118.1*, 135.8# | This Calc. |
| $Ti_2SiC$ | 267.7* , 300.1# | 69.8 *, 83.5# | 90.9* , 105.7# | 289.4* , 313.5# | 120.1* , 153.6# | This Calc. |

***** *Shows results obtained from QE*
*# shows those obtained from VASP*

Table 3 shows elastic anisotropies for the nine $M_2AX$ MAX phase materials. It is noted that $A_2$ is greater than $A_1$ for all the materials, denoting that it is easier to compress these $M_2AX$ materials in any direction perpendicular to the hexagonal axis.

**Table 3:**

*Calculated Elastic Anisotropies A1 and A2 for Ti2AlC, Ti2AlN, Ti2GaC, Ti2GaN, Ti2PbC, Ti2CdC, Ti2SnC, Ti2GeC and Ti2SiC MAX Phases*

| | | Anisotropies for Hexagonal materials Under study | | |
|---|---|---|---|---|
| S/No | Phase | $A_1$ | $A_2$ | Remarks |
| 1 | $Ti_2AlC$ | 0.0028 | 0.0052 | $A_2 > A_1$ |
| 2 | $Ti_2AlN$ | 0.0019 | 0.0042 | $A_2 > A_1$ |
| 3 | $Ti_2GaC$ | 0.0034 | 0.0059 | $A_2 > A_1$ |
| 4 | $Ti_2GaN$ | 0.0022 | 0.0047 | $A_2 > A_1$ |
| 5 | $Ti_2CdC$ | 0.0064 | 0.0066 | $A_2 > A_1$ |
| 6 | $Ti_2PbC$ | 0.0042 | 0.0085 | $A_2 > A_1$ |
| 7 | $Ti_2SnC$ | 0.0036 | 0.0070 | $A_2 > A_1$ |
| 8 | $Ti_2GeC$ | 0.0018 | 0.0043 | $A_2 > A_1$ |
| 9 | $Ti_2SiC$ | 0.0017 | 0.0042 | $A_2 > A_1$ |

The calculated values of elastic moduli; bulk modulus *B*, shear modulus *G*, Young modulus *E* and Poisson's ratio *v* of the considered MAX phase compounds obtained using the Voigt-Reuss-Hill approximation (Hill, 1952) are shown in Table 4.

**Table 4:**

*Calculated Elastic Moduli B, G, E (Gpa) and N for Ti2AlC, Ti2AlN, Ti2GaC, Ti2GaN, Ti2PbC, Ti2CdC, Ti2SnC, Ti2SiC and Ti2GeC MAX Phases Obtained Using VASP and QE Codes Compared with Available Theoretical and Experimental Data*

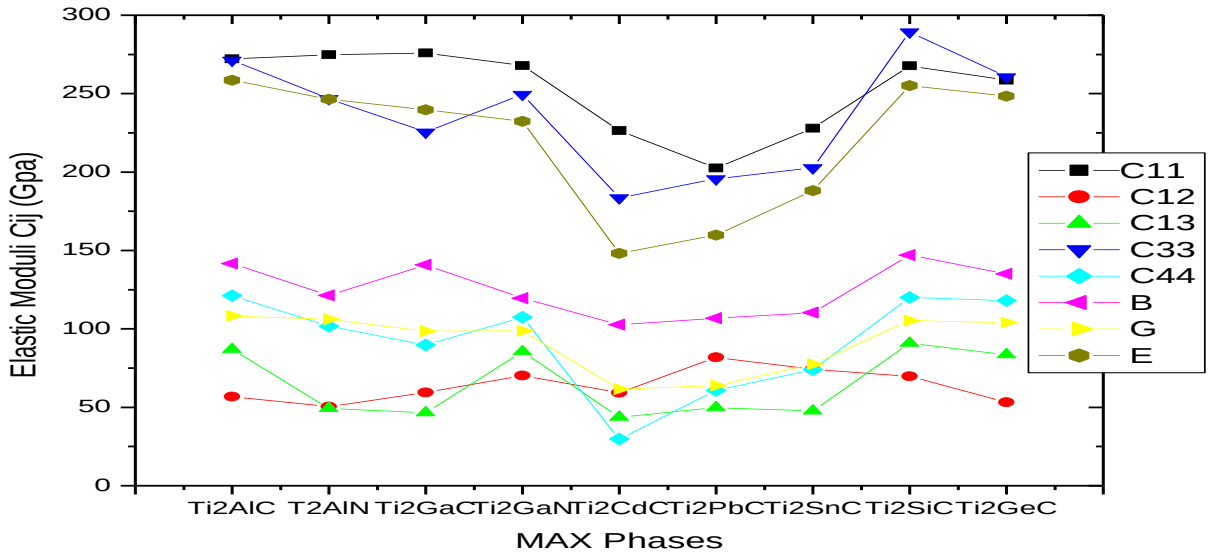
| | *B* | *G* | *E* | *B/C*$_{44}$ | *B/G* | *v* | Reference |
|---|---|---|---|---|---|---|---|
| $Ti_2AlN$ | 141.7*,155.1# | 108.2*, 126# | 258.6*,277.3# | 1.17*,1.31# | 1.23*,1.31# | 0.19*, 0.2# | This Calc. |
| | 162.55 | 126 | 300 | 1.32 | 1.29 | 0.192 | (Rahaman *et al.*, 2015) |
| | 177 | 127 | 307 | 1.42 | 1.39 | - | ( Cover, 2008), |
| $Ti_2AlC$ | 121.4*,136.1# | 106.1*, 115# | 246.5 , 267# | 1.19*,1.24# | 1.14*, 1.18# | 0.16*,0.17# | This Calc. |
| | 137 | 117 | 273 | 1.20 | 1.15 | 0.164 | (Du et al, 2009). |
| | 138 | 113 | 267 | 1.27 | 1.22 | - | ( Cover, 2008), |
| $Ti_2GaC$ | 140.8*,153.6# | 98.6 *, 108.2# | 239.8*,263.5# | 1.31*,1.35# | 1.42*, 1.43# | 0.17*,0.22# | This Calc. |
| | 140.88 | 121 | 283 | 1.20 | 1.16 | 0.166 | (Rahaman *et al.*, 2015) |
| $Ti_2GaN$ | 119.5*,138.8# | 98.8*, 110.5# | 232.3*, 262# | 1.23*,1.33# | 1.21*,1.26# | 0.18*,0.19# | This Calc. |
| | 181 | 122 | 300 | 1.33 | 1.48 | 0.22 | LDA (Bouhemadou, 2009) |
| | 156 | 108 | 264 | 1.44 | 1.32 | 0.218 | GGA (Bouhemadou, 2009) |
| $Ti_2SnC$ | 110.3*,137.2# | 77.4*, 93# | 188.2*, 228# | 1.49*, 1.51# | 1.42* ,1.48# | 0.22 | This Calc. |
| | 134.44 | 93 | 226 | 1.45 | 1.45 | 0.218 | (Rahaman *et al.*, 2015) |
| $Ti_2CdC$ | 102.6*,113.5# | 61.5*, 65# | 148.2*, 153.# | 2.85*,3.81# | 1.67*,1.75# | 0.24*,0.25# | This Calc. |
| | 115.66 | 69.6 | 174 | 3.51 | 1.66 | 0.249 | (Rahaman *et al.*, 2015) |
| $Ti_2PbC$ | 106.7*,118.9# | 63.9*, 74# | 159.8*,183.9# | 1.75*,1.83# | 1.61*,1.67# | 0.24 *,0.25# | This Calc. |
| | 119.22 | 73.2 | 182 | 1.81 | 1.63 | 0.245 | (Rahaman *et al.*, 2015) |
| $Ti_2SiC$ | 147.1*,166.8# | 105.3*,122.1# | 255.2*,294.5# | 1.13*,1.22# | 1.37*,1.40# | 0.2*, 0.21# | This Calc. |
| $Ti_2GeC$ | 135.1*,154.6# | 104.0*,111.6# | 248.4*,269.9# | 1.09*,1.14# | 1.30*,1.39# | 0.20*, 0.21# | This Calc. |

** Shows results obtained from QE*
*# shows those obtained from VASP*

Figure 4 below shows a plot of the calculated elastic and mechanical properties of the nine $Ti_2AX$ MAX phase materials.

**Figure 4:**

*Elastic Constants with (A) Bulk Modulus (B), Shear Modulus (G), Young's Modulus (E), Machinability Index B/C44), Ductility Index (B/G) And Poisons Ratio (N)*

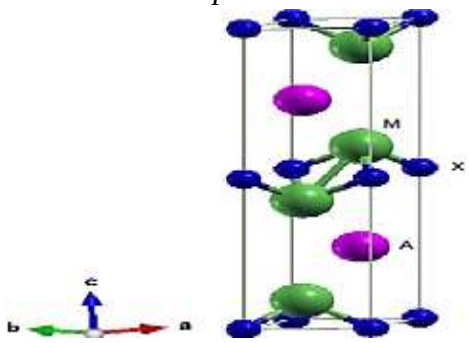


## IV. DISCUSSION

These properties were computed primarily as a validation of the correct structures from which the structural and elastic properties were obtained. As mentioned earlier, the $M_2AX$ materials usually crystallize in the hexagonal structure with the space group P63/mmc no. 194. The unit cell structure of $M_2AX$ compounds is shown in Figure 5 and it comprises of 2 formula units with 8 atoms. The calculated equilibrium lattice parameters, such as the lattice constants a, c, and c/a of the MAX phases are shown in Table 1. The computed lattice parameters show good agreement with other theoretical data and careful look at the calculated lattice parameter, c, obtained from both QE and VASP codes show that the results deviate from experimental data by less than an overall error of ± 2% except for $Ti_2AlN$ where the calculated value of a was within <4% margin of error compared to the corresponding experimental values.

**Figure 5:**

*Crystal Structure of the 211 M2AX Phase Compounds*




The green ball represents the M (Ti) atoms, Violet ball stands for the A atom (A = Al, Ga, Sn, Cd, Pb, Si and Ge) and the blue ball represents X atoms (X = C or N).

The structures show that they all possess the expected hexagonal structures, with the Ti atom bonded to three C or N atoms. The bond lengths and lattice parameters were then plotted against the respective materials as shown in Fig 2 and 3 respectively. Fig 2 shows that the nine materials have longer bond lengths between the X-X elements averaging around 3.2 Å. This shows that the bond is weaker compared to the shorter and stronger bond lengths between Ti-X averaging around 2.12Å. The calculated bond lengths of these materials are in good agreement with the available experimental values and other theoretical investigations.

The optimized values of the 'c' parameter are higher than the values of 'a' as shown in Fig 3 and this agrees well with the available experimental and theoretical studies (Atikur, 2015; Magnuson, 2017). The lower curve is almost flat showing that the 'a' parameters were quite close to each other, with minimal deviations of about 0.209Å. The upper curve shows a wider spread in the calculated values of the **c** parameter, with the shortest value being 12.88Å for $Ti_2SiC$ and the longest value was 14.45Å for $Ti_2CdC$. Nonetheless, the values were still in agreement with the other available experimental and theoretical studies.

The mechanical behaviour of solids which governs their use largely depends upon their elastic constants. Table 2 shows the computed values of the elastic constants for the nine MAX phase materials considered in this study. The elastic constants provide vital information on the stability, stiffness, brittleness, ductility, and elastic anisotropy of a given material. Since MAX phases

possess hexagonal crystal structures (Rahaman *et al.*, 2015; Anirudh, 2014), they have five independent elastic constants: $C_{11}$, $C_{12}$, $C_{13}$, $C_{33}$ and $C_{44}$. A mechanically stable MAX phase compound should obey the following stability conditions (Beckstein et al., 2001; Wallace, 1972; Birch, 1947): $C_{11} > 0$, $C_{33} > 0$, $C_{44} > 0$, $(C_{12} - C_{12}) > 0$, and $(C_{11} + C_{12})\, C_{33} > 2(C_{12})^2$.

The predicted elastic constants for the nine MAX phase materials are found to be in good agreement with the available theoretical data (Bai *et al.*, 2010; Cover *et al.*, 2008; Sun *et al.*, 2008; Bouhemadou & Khenata, 2007; Holm *et al.*, 2002). The estimated elastic constants are positive and obey the well-established Born stability conditions (Beckstein *et al.*, 2001; Wallace, 1972; Birch, 1947), which therefore confirms that the studied MAX phase compounds are indeed mechanically stable at ground-state conditions 'and as such, forms a good foundation for their study at elevated temperatures'. It is also observed that $C_{11} > C_{33}$ (see Table 2), implying that the compounds are highly compressible along the *c*-direction. It also indicates that the compounds are elastically anisotropic.

The results of this study agree quite well with other theoretical values except those from (Kanoun *et al.*, 2009, Liu *et al.*, 2009) which show that $C_{33} > C_{11}$ suggesting that the *c*-axis is the least compressible. On the other hand, it is evident from Table 2 that the calculated range of elastic constants such as, $C_{11}$, $C_{33}$ and $C_{44}$ for $Ti_2SnC$ are significantly smaller than those obtained by Kanoun *et al.* (2009) and Bouhemadou *et al*. (2008) and all were obtained from first principles based on density functional theory. This variance could be resulting from the slight difference in the structural optimization values, and to a smaller extend the pseudopotentials used in the two codes. Overall, and as seen from Table 2, the elastic constant $C_{11}$ is seen to decrease as: $Ti_2GaN$ > $Ti_2AlC$ > $Ti_2AlN$ > $Ti_2GaN$ > $Ti_2SiC$ > $Ti_2GeC$ > $Ti_2SnC$ > $Ti_2CdC$ > $Ti_2PbC$. The $C_{12}$ elastic constant at the same time decreases following the order $Ti_2PbC$ > $Ti_2SnC$ > $Ti_2GaN$ > $Ti_2SiC$ > $Ti_2GaC$ > $Ti_2CdC$ > $Ti_2AlN$ > $Ti_2GeC$ > $Ti_2AlC$. Similarly, the elastic constant $C_{13}$ adopts the following trend: $Ti_2SiC$ > $Ti_2AlN$ > $Ti_2GaN$ > $Ti_2GeC$ > $Ti_2PbC$ > $Ti_2AlC$ > $Ti_2SnC$ > $Ti_2GaC$ > $Ti_2CdC$. As for the $C_{33}$, trend follows: $Ti_2SiC$ > $Ti_2AlN$ > $Ti_2GeC$ > $Ti_2GaN$ > $Ti_2AlC$ > $Ti_2GaC$ > $Ti_2SnC$ > $Ti_2PbC$ > $Ti_2CdC$ while the $C_{44}$ elastic constant has $Ti_2AlN$ with highest value and $Ti_2CdC$ having the smallest value. Comparing the nine MAX phase materials, one notes that their $C_{44}$ elastic constants decreases using the trend: $Ti_2AlN$ > $Ti_2SiC$ > $Ti_2GeC$ > $Ti_2GaN$ > $Ti_2AlC$ > $Ti_2GaC$ > $Ti_2SnC$ > $Ti_2PbC$ > $Ti_2CdC$. From the $C_{11}$ values, it was discovered that $Ti_2GaN$ had the highest value with $Ti_2PbC$ having the smallest. Similarly, $Ti_2AlC$ was found to possess the smallest value with $Ti_2PbC$ having the highest with respect to $C_{12}$. As for the $C_{13}$ and $C_{33}$, $Ti_2SiC$ possessed the highest value with $Ti_2CdC$ having the least in both cases. On the other hand, $Ti_2AlN$ had the highest while $Ti_2CdC$ had the smallest value with reference to $C_{44}$.

Table 3 shows the calculated elastic anisotropy factors of the nine $M_2AX$ phase materials. The elastic anisotropy factor, *A*, determines how the elastic properties of a solid are dependent on the direction of the stress. Moreover, the elastic anisotropy is also connected with the thermal expansion and the crystal micro- cracks (Sun *et al*, 2004). For the MAX phase systems that are hexagonal, the elastic anisotropy factor is calculated from the expression $A = 4C_{44} / (C_{11} + C_{33} - 2C_{13})$, and if $A = 1$, the crystal is isotropic while any value smaller or lager than 1 indicates anisotropy. The results from Table 3 indicate that all the studied $M_2AX$ phase materials are elastically anisotropic, which agrees well with other theoretical predictions (Zhuangzhuang *et al.*, 2019). Moreover, $Ti_2CdC$ is considered more anisotropic compared to the other studied

compounds by virtue of the calculated A value. This value limits the application of these materials since it is applied in determining the parameters of interest like machinability and others required for industrial application.

Bulk and shear moduli are important parameters used to estimate the hardness of a material. Out of the nine MAX phase compounds, $Ti_2CdC$ is found to possess the smallest value of bulk (102.6Gpa) and shear modulus (61.5Gpa), which implies that it is a highly compressible material. This is consistent with the property of the material that it is the most anisotropic as mentioned earlier. It is further noted that the calculated bulk and shear moduli data agree quite well with other available theoretical and experimental studies (especially for $Ti_2AlC$) with a percentage deviation of approximately 1.57% (Gilles & Evelyne, 2002).

Young's modulus (*E*) is an indicator of the stiffness of a material, so that, the larger the value of *E*, the stiffer the material and vice versa. The findings of this study show that $Ti_2AlN$ has the highest value (258.8Gpa) of *E* while $Ti_2CdC$ has the lowest (148.2Gpa), indicating that $Ti_2AlN$ is the stiffest among the nine materials (see Table 4). This is equally in line with the observed anisotropies where $Ti_2AlN$ has the largest value of 1.26 while $Ti_2CdC$ has the lowest of 0.33. The Poisson's ratio, *v*, assesses the nature of chemical bonding in solid materials (Savin *et al.*, 1992), with the values for pure covalent and ionic crystal being, 0.1 and 0.25 respectively. The results of the Poisson's ratio for the studied materials lies between these two characteristic values, indicating that the compounds possess a mixture of both covalent and ionic bonding, which gives them the observed high values of hardness and stiffness. According to Pugh's ratio (*B/G*) (Pugh, 1954), a material is ductile if $B/G > 1.75$; otherwise, it is brittle. The calculated *B/G* values (see Table 4) show that the $Ti_2MX$ MAX phase materials under study are brittle in nature which is consistent with the general behaviour of MAX phases (Liu *et al.*, 2009; Cover *et al.*, 2008; Wang & Zhou, 2004).

Table 4 shows the calculated indices for machinability, defined as $B/C_{44}$ (Sun, 2005; Sun *et al.*, 2003) and ductility, defined as B/G (Sun *et al.*, 2003; Pugh, 1954). The table gives very important information into the relative roles of the nitrides and carbides slab and the A element in determining the elastic properties and related macroscopic consequences of these MAX phase materials. The important macroscopic properties that depend on the elastic constants are the machinability and ductility. From Table 4 it is seen that machinability of the materials understudy decreases in the following order with their corresponding machinability index in bracket: $Ti_2CdC$ (2.6), $Ti_2PbC$ (1.8), $Ti_2SnC$ (1.5), $Ti_2GaC$ (1.3), $Ti_2GaN$ (1.3), $Ti_2SiC$ (1.2), $Ti_2AlC$ (1.2), $Ti_2AlN$ (1.2) and $Ti_2GeC$ (1.1). Out of this, it is noted that $Ti_2CdC$ has the highest value while $Ti_2Gec$ has the least. Therefore, in areas where high machinability is required, then $Ti_2CdC$ will be the most preferred.

The ductility measured by B/G values, show that the nitrides and carbides do not have significant difference in their ductility. Their ductility indices decrease in the following order with their respective values in bracket, $Ti_2PbC$ (1.6), $Ti_2CdC$ (1.6), $Ti_2GaN$ (1.4), $Ti_2SnC$ (1.4), $Ti_2SiC$ (1.3), $Ti_2AlN$ (1.3), $Ti_2GeC$ (1.2) $Ti_2GaC$ (1.2) and $Ti_2AlC$ (1.1). From this findings, it was found that $Ti_2AlC$ had the least value with $Ti_2PbC$ and $Ti_2CdC$ having the highest ductility index. In areas where ductility is, required then $Ti_2PbC$ and $Ti_2CdC$ will be significant.

From Fig 4 it is noted that $C_{11}$ has the highest values followed by $C_{33}$, E, B. The other parameters $C_{44}$, G, $C_{13}$ and $C_{12}$ show some fluctuations of about 24 % from the respective average values. Notably, there is a general decrease in the values as larger A elements are included into the compound from Cd, Pb and Sn. This suggests that the large elements tend to marginally compromise the elastic and mechanical properties of the respective compounds. The other indicators B/$C_{44}$, B/G and n has the low values which are close to unity. It's also worth noting that the values obtained in this study are in agreement with the values obtained by other researchers as referenced Table 3.

## Conclusion

The findings of this study have established that all the nine Max phase compounds possess the hexagonal structure with the X-X bond lengths being longer than the Ti-X, Ti-Ti and Ti-Ga bonds. The lattice parameters were equally in good agreement with other studies to within a margin of error of 1.46% and 1.14% for the cell parameters *'a'* and '*c'* respectively. The ratio c/a was found to vary from 4.33 to 4.66 for all the materials studied. The calculated bulk modulus showed $Ti_2CdC$ having the smallest value of 102.6 Gpa, while $Ti_2SiC$ had the highest value of 147.1 Gpa. It's also noted that $Ti_2CdC$ has the smallest value of the shear modulus of 61.5 Gpa while $Ti_2AlN$ has the highest value of 108.2 Gpa. In a case where twisting and turning is of paramount importance then $Ti_2AlN$ will be preferred, due to its large value of shear modulus. $Ti_2CdC$ was also found to have the smallest value of the young's moduli of 148.2 Gpa while $Ti_2AlN$ was found to have the highest value of 258.6 Gpa. This suggest that $Ti_2AlN$ is the stiffest among the nine Ti based MAX phase compounds considered in this study and $Ti_2CdC$ is the most plastic. The machinability index, B/$C_{44}$ shows that $Ti_2GeC$ has the smallest value of 1.09 while $Ti_2CdC$ has the highest value of 2.85. In a case where highly machinable material is required then $Ti_2CdC$ will be the choice. In terms of ductility index, B/G, $Ti_2AlC$ has the lowest value of 1.14 while $Ti_2CdC$ has the highest value of 1.67 and in a situation where ductility is required then $Ti_2CdC$ is the most preferred material. According to Pugh's ratio (B/G), a material is ductile if B/G > 1.75; otherwise, it is brittle. These values show that the nine $M_2AX$ phase materials under study are brittle in nature with $Ti_2PbC$ and $Ti_2CdC$ being more brittle and $Ti_2AlC$ being the least. This explains partly why the MAX Phases are also easily machinable.

As for the poison ratio, it was found that $Ti_2AlC$ had the lowest value of 0.16 while $Ti_2CdC$ and $Ti_2PbC$ had similar highest value of 0.24. The results of the elastic constants determined in this study agree quite well with other theoretical values. In particular, $C_{11}$ is largest in $Ti_2AlN$ at 308.4Gpa while $C_{12}$ is largest for $Ti_2PbC$ at 90.6Gpa. The elastic constants $C_{12}$, $C_{33}$ and $C_{44}$ were found to have the largest values for $Ti_2SiC$ at 105.7Gpa, 313.5Gpa and 153.6Gpa respectively. The calculated elastic and mechanical properties predicted that all the nine MAX phase compounds were indeed suitable for various industrial applications ranging from machining, twisting and turning, especially due to their relatively low hardness compared to other traditional hard materials like boron nitride and diamond.

**Recommendations**

The most urgent issue in MAX phase materials is to come up with viable commercial applications for these compounds especially now that they have already been established to have very many desirable properties. New and novel MAX phases and higher order materials with their applications need to be ventured into in order to meet the growing demand for there is need to combine modelling and experimental approaches to synthesize the desired materials. This study determined from first principle approaches the mechanical and elastic properties of nine $Ti_2AX$ phase materials that can be used in industry and hence techniques need to be developed to realize the materials in more affordable way.

This study has considered a group of Ti MAX Phases with specifically n=1, their properties and a variety of applications for different industrial applications. It is expected that this study will be of great importance in establishing a firm foundation for the development of novel MAX Phase compounds. Their practical and possible applications in the coming days especially with the advancement in technology to meet the industrial needs will be of greater value to the world.

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