Electronic and Lattice Dynamical Properties of Ti_2SiB MAX Phase

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Abstract

The structural, electronic, mechanic, vibrational and thermodynamic properties of Ti_2SiB which is a hypothetical MAX phase compound, have been investigated using density functional theory calculations. The structural optimization of Ti_2SiB has been performed and the results have been compared with Ti_2SiC, Ti_2SiN, and Ti_2AlB that are studied in the literature. Then the band structure and corresponding partial density of states are computed. In addition, charge density and Bader charge analysis have been performed. The elastic constants have been obtained, then the secondary results such as bulk modulus, shear modulus, Young's modulus, Poisson's ratio, and Vickers Hardness of polycrystalline aggregates have been derived, and the relevant mechanical properties have been discussed. Moreover, the elastic anisotropy has been visualized in detail by plotting the directional dependence of compressibility, Poisson ratio, Young's and Shear moduli. Furthermore, the phonon dispersion curves as well as corresponding phonon PDOS, and thermodynamical properties such as free energy, entropy and heat capacity have been computed and the obtained results have been discussed in detail. This study provides the first considerations of Ti_2SiB that could have a potential application in nuclear industry.

Keywords: MAX phases; Ti_2SiB; electronic properties; mechanical properties; phonon; Bader charge analysis

1. Introduction

MAX phases have $M_{(n+1)}AX_n$ formula with n=1,2 and 3 where M is a transition metal, A is an A group element and X is Carbon and/or Nitrogen [1]. The MAX phases crystallize in $P6_3/mmc$ hexagonal structure and their ionic, metallic and covalent bonding give them unique properties [2]. The MAX phases have both metallic and ceramic properties that lead to good damage tolerance, high strength and stiffness at high temperatures, good

electrical and thermal conductivity and good corrosion resistance [3–5]. Owing to these properties, the MAX phases can be implemented for applications such as wear and corrosion resistant coatings [6], superconducting materials [7], and nuclear industry [8].

The MAX phases are studied experimentally, for example, Hu et al. [9] fabricated Nb_4AlC_3 using spark plasma sintering and investigated its thermal expansion and electrical conductivity and Barsoum and Radorovic [5] reviewed the results of the measurement of elastic properties of some selected MAX phases. Also, theoretical study of MAX phases are available in the literature, for example, Bouhemadou and Khenata [10] studied the structural, elastic and electronic properties of M_2SC (M=*Ti, Zr, Hf*) and He et al. [11] studied the lattice constants, Bulk modulus, band structure and partial density of states for Ti_2InC, Zr_2InC, and Hf_2InC. The given studies are examples and there are many studies for MAX phases. Furthermore, studies of the MAX phases are focused on different combinations of M- and A- site atoms and X site atom is kept C and/or N [2]. Recently, MXenes which are 2D materials, are layered MAX phases and has been investigated to explore their properties[12]. Moreover, the MAX phases of Ti_3SiC_2, Ti_3AlC_2 and Ti_2AlC have been examined how they behave under neutron radiation [13] and they are radiation hard similar to SiC which is one of the most used material in nuclear reactors. On the other hand, Borides of MAX phases would be an alternative new material for control rods at nuclear reactors due to having the high neutron cross section of Boron. Moreover, Borides of MAX phases would be used in nuclear industry due to their stability. There are very few studies that have X site as Boron [14–16] and therefore, the aim of this study is to determine the properties of Ti_2SiB compound which has Boron for X site atom and could have potential application in nuclear industry.

In this study, Ti_2SiB is investigated for the first time as we know up to date and compared with Ti_2SiC and Ti_2SiN that are detailed studied in the literature [17–27] and also Ti_2AlB from a previous study [15]. Calculation details for Ti_2SiB are illustrated in Section 2. The structural optimization results, electronic properties and charge density analysis of Ti_2SiB are presented in Section 3. The calculated formation enthalpy indicates that Ti_2SiB is a stable phase. After these results, mechanical properties such as elastic constants, bulk modulus, shear modulus, etc. are detailed in Section 4. The phonon band structure and thermodynamic properties are presented

in Section 5 where the Raman modes are also included. Finally, the study concludes with a brief summary in Section 6.

2. Calculation Details

The DFT calculations are performed using the Vienna Ab initio Simulation Package (VASP) [28]. The pseudopotentials are chosen according to Perdew-Burke-Ernzerhof (PBE) parametrization of the generalized gradient approximation (GGA) for the exchange and correlation terms of the electron-electron interaction [29]. For the electron-ion interaction, Projector Augmented Wave (PAW) method [30] has been implemented and the kinetic energy cut off is chosen 500 eV. The 16 x 16 x 4 k-point mesh has been generated which is centered at the Γ- point. The electronic energy change is kept 10^{-11} eV. The structure is optimized with the minimization of the stresses and the Hellman-Feynman forces. The elastic constants are calculated using the stress-strain method with VASP. The anisotropic elastic properties are obtained with ELATE program [31] where the calculated elastic constants are employed. The phonon calculations are performed for a 2 x 2 x 1 supercell with the Phonopy code [32].

3. Structural Optimization and Electronic Properties

The lattice structure of Ti_2SiB compound which belongs to the space group of 194 ($P6_3/mmc$) is given in Figure 1. The *Ti* atoms are interleaved with the *Si* atoms and the octahedral sides are filled with the *B* atoms as shown in Figure 1. The *Ti* atoms occupy at 4f, the *Si* atoms occupy at 2d and the *B* atoms occupy at 2a Wyckoff positions.

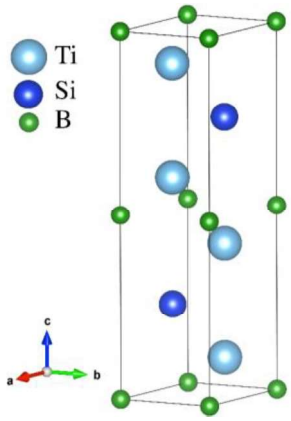

Figure 1. The lattice structure of Ti_2SiB compound

Lattice parameters, formation energy and z parameter of the Wyckoff positions of the *Ti_2SiB* compound are given in Table 1 and the results from the literature for *Ti_2SiC* [22,24], *Ti_2SiN* [17,26] and *Ti_2AlB* [15] are also listed. The lattice parameters are increasing when the *X* atom goes from nitrogen to boron for *Ti_2SiX* as can be seen in Table 1. Once *Ti_2SiB* and *Ti_2AlB* are compared, c parameter of *Ti_2AlB* is around 8% higher than that of *Ti_2SiB*. The *Ti_2SiB* compound is hypothetical therefore there is no experimental data nor theoretical study in order to compare the calculation results. The formation energy is calculated using Equation 1 and negative formation energy indicates that the compound is thermodynamically stable. Hence, the results specify that these compounds can be synthesized.

$$E_{Formation} = E_{Ti_{2SiB}} - 2E_{Ti} - E_{Si} - E_B \quad (1)$$

Table 1. Lattice parameters, formation energy and z parameter of the Wyckoff positions of the Ti_2SiB, Ti_2SiC and Ti_2SiN compounds

Material	Reference	a (Å)	c (Å)	ΔH_f(eV/atom)	z
Ti_2SiB	This study	3.151	12.979	-3.972	0.095
Ti_2SiC	Theory [22]	3.052	12.873	-	0.092
Ti_2SiC	Theory [24]	3.052	12,873	-0.860	0.092
Ti_2SiN	Theory [17]	2.979	12.82	-	0.093
Ti_2SiN	Theory [26]	2.984	12.822	-	0.093
Ti_2AlB	Theory [15]	3.148	14.064	-3.577	0.087

The band structure for *Ti_2SiB* is predicted along the high symmetry directions in the first Brillouin zone from the calculated equilibrium lattice constant. The band structures and corresponding partial and total electronic density of state (DOS) are displayed drawn and given in Figure 2 and Figure 3, respectively.

It is clear that the compound is metallic due to the fact that the DOS values differ from zero at the Fermi level.

The most significant contribution to PDOS comes from the s states of *B* and *Si* atoms between -7 eV and -5 eV energy range and from d states of *Ti* between -2 eV and 3 eV energy range as seen in Figure 3.

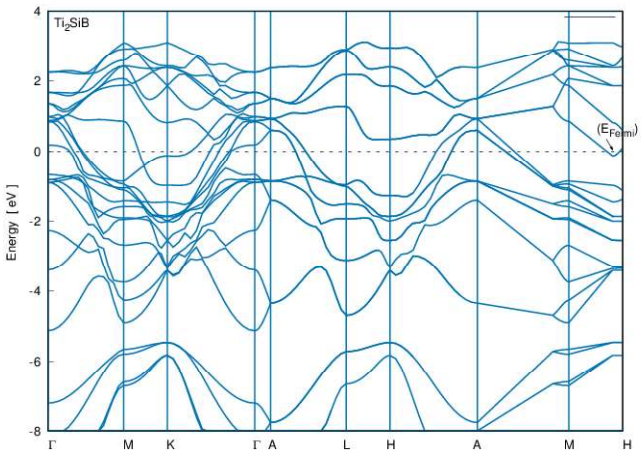

Figure 2. Band structure of Ti_2SiB

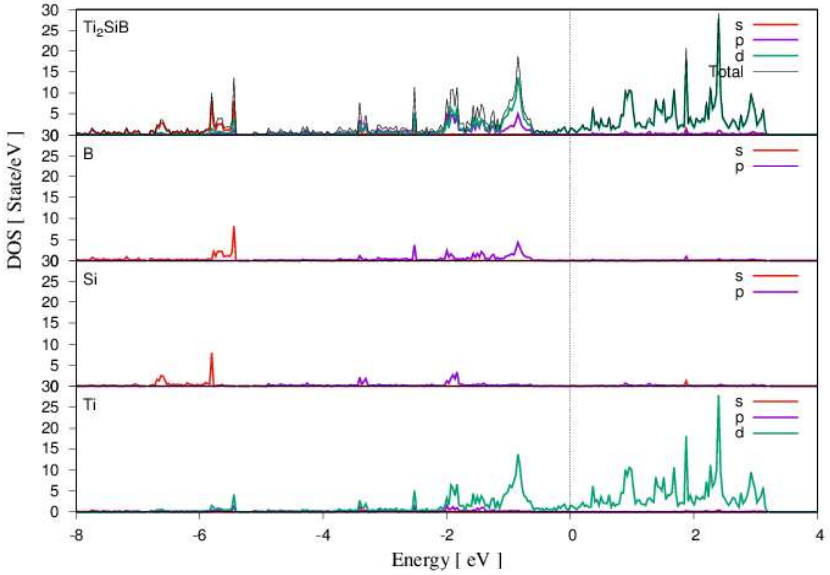

Figure 3. Partial density of states of Ti_2SiB

After these electronic structure calculations, the charge density and bader charge analysis is performed in order to determine the bonding nature and charge of the ions for *Ti_2SiB*. The charge density plot of *Ti_2SiB* indicates that *Ti_2SiB* has dominantly ionic bonding as shown in Figure 4. Bader charge population analysis is also performed in order to get the bonding nature of *Ti_2SiB*. The calculation is performed with VASP and analysis is

performed using the algorithm developed by Henkelman et. al. [33] which is based on Bader's suggestion [34]. Table 2 lists the Bader net charge of the ions for *Ti_2SiB*. If the Bader net charge is positive, the charge is transferred away from the atom, vice versa for the negative Bader net charge [35]. The charge is transferred away from *Ti* atom, while the charge is transferred to *Si* and *B* atoms. The bond length of *Ti-Si* is 2.712 Å and it is 2.198 Å for *Ti-B*.

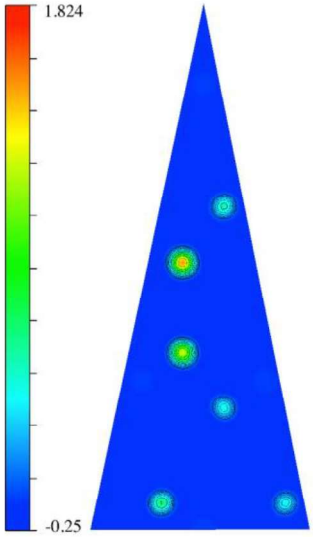

Figure 4. The charge density of Ti_2SiB compound

Table 2: Bader net charge of the atoms for Ti_2SiB in units of e

Atom	Bader Charge
Ti	0.552
Si	-0.282
B	-0.822

4. Mechanical Properties

Mechanical properties of *Ti_2SiB* are investigated after the structural optimization. The elastic constants (C_{ij}) are calculated using the stress-strain method with VASP which are listed in Table 3. In addition, to compare the obtained results with the literature, the table contains the results for *Ti_2SiC* [22,24], *Ti_2SiN* [17,26] , and *Ti_2AlB* [15] . Also, the elastic constants of *Ti_2SiB* has lower value when compared to the values of *Ti_2SiC and Ti_2SiN*. On the other hand, this value is higher than the value given for *Ti_2AlB*. The stability of *Ti_2SiB* are determined using Born stability criteria [36] and found that it is mechanically

stable.

Table 3: The calculated elastic constants (in GPA) of the Ti_2SiB and results for Ti_2SiC and Ti_2SiN taken from the literature

Material	Reference	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
Ti_2SiB	This study	250.1	74.8	80.9	262.8	119.6
Ti_2SiC	Theory [23]	311.4	85.8	111.5	324.2	146.1
Ti_2SiC	Theory [19]	311.0	84.0	107.0	343.0	155.0
Ti_2SiN	Theory [17]	298.0	96.0	127.0	347.0	153.0
Ti_2SiN	Theory [26]	296.7	100.2	126.3	347.8	155.1
Ti_2AlB	Theory [15]	234.0	73.9	80.6	261.9	115.1

The mechanical properties of *Ti_2SiB*, which are obtained with the calculation of the elastic constants, are listed in Table 4. The literature results for *Ti_2SiC* and *Ti_2SiN* are also given in Table 4. The Bulk modulus (B) and the shear modulus (G) are calculated with the Voigt-Reuss-Hill approximations [37–39]. Voight approximation gives the lower limit while Reuss approximation gives the upper limit of these moduli. Hill approximation takes the average of the Voigt and Reuss results which is generally consistent with the experimental results. As it is well known that Bulk modulus (B) is the volume change of a material if there is a stress on it. So, it defines the incompressibility of a material. The Bulk modulus of *Ti_2SiX* compound increases when *X* element goes from Boron to Nitrogen. On the other hand, if *Ti_2SiB* and *Ti_2AlB* are compared, *Ti_2AlB* has higher Bulk modulus then *Ti_2SiB*. Shear modulus (G) is also known as the length change of a material when a shear stress is applied. So, it is a measure of the resistance of the transverse deformations. Once the Shear modulus of *Ti_2SiB* compound is compared, it has lower Bulk modulus than that of *Ti_2SiC and Ti_2SiN* while it has higher Bulk modulus than *Ti_2AlB*. Young's modulus (E) is defined as the length change of a material when a pull or push is applied. It is also called modulus of elasticity. Young's modulus of *Ti_2SiB* shows similar behavior with the Shear modulus. Poisson's ratio (ϑ) is the ratio of the transverse strain to axial strain. It is used to determine the bonding characteristics of a material. The material has ionic bonding if ϑ is around 0.25 while if ϑ is small around 0.1, it has covalent

bonding [40]. ϑ value of *Ti_2SiB* compound indicates that it has dominantly ionic bonding. Also, the literature results for *Ti_2SiC, Ti_2SiN and Ti_2AlB* show that they both have dominantly ionic bonding. B/G ratio determines the ductility or brittleness of a material and if it is higher than 1.75, the material is ductility, otherwise, it is brittle [41,42]. *Ti_2SiB* compound is brittle that can be inferred from B/G ratio of it. G/B ratio is called Pugh's modulus and it is used to determine the bonding nature of a material. If G/B is around 1.1, the material has dominantly covalent bonding [40]. On the other hand, the ionic character is dominant if G/B ratio is around 0.6 [40]. *Ti_2SiB* compound has dominantly ionic bonding as can be concluded from G/B ratio which is consistent with the results from ϑ value and the charge density analysis. The hardness of *Ti_2SiB* is also calculated using Chen et. al. approach [43]. As shown in Table 4, *Ti_2SiB* has the hardness (17.6 GPa) value that is higher than the value given for *Ti_2AlB (16.3 GPa).* Thus, *Ti_2SiB* could be considered as the hard material.

Table 4: The calculated mechanical properties (Bulk Modulus – B (in GPa), Shear modulus – G (in GPa), Young's modulus - E (in GPa), Poisson's ratio – ϑ, B/G ratio, G/B ratio, Vicker's hardness - H_v (in GPa)) of Ti_2SiB and Ti_2SiC and Ti_2SiN taken from literature.

Material	Reference	B	G	E	ϑ	B/G	G/B	H_v
Ti_2SiB	This study	137.2	99.3	239.9	0.208	1.381	0.723	17.6
Ti_2SiC	Theory [23]	173.6	122.0	296.6	0.215	-	0.70	-
Ti_2SiC	Theory [19]	172.5	128.5	309	0.20	1.34	-	-
Ti_2SiN	Theory [17]	182	118	291	0.233	-	-	-
Ti_2SiN	Theory [26]	181.9	117.8	290.7	0.234	-	-	-
Ti_2AlB	Theory [15]	134.0	93.6	227.4	0.215	1.420	0.703	16.3

The anisotropic elastic properties are studied because this calculation is important in order to complete the elastic properties of a material. The anisotropic properties provide to determine some material properties under a plastic deformation or dislocation dynamics. The anisotropy is higher if the spherical shape is distorted. The elastic stiffness matrix is calculated using VASP. This matrix is employed to ELATE program [31]. Figure 5 shows Young's modulus, linear compressibility, Shear modulus and Poisson's ratio in xy, xz and yz planes. The green curves show the minimum and the blue curves

show the maximum points for the parameters. The maximum and minimum values for these parameters are given in Table 5. Furthermore, the results for *Ti_2AlB* [15] are also listed in Table 5 as well. Young's modulus and linear compressibility are isotropic in all planes. Shear modulus and Poisson's ratio are anisotropic in xy and xz planes, while they are isotropic in yz plane.

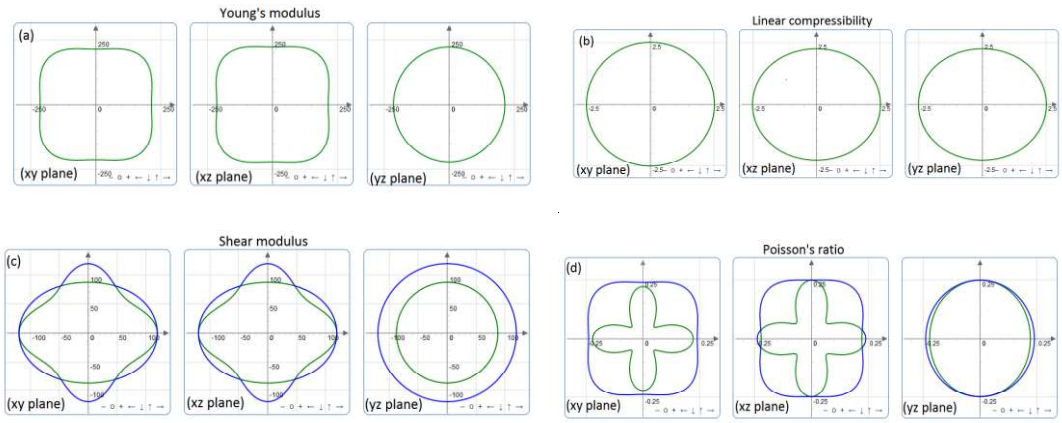

Figure 5. Young's modulus (a), linear compressibility (b), Shear modulus (c) and Poisson's ratio (d) in xy, xz and yz planes for Ti_2SiB

Table 5: The maximum and minimum values of Young's modulus (E, in GPa), linear compressibility (β), shear modulus (G, in GPa) and Poisson's ratio (ϑ) of Ti_2SiB

	Reference	Young's modulus		Linear compressibility		Shear Modulus		Poisson's ratio	
		E_{min}	E_{max}	β_{min}	β_{max}	G_{min}	G_{max}	ϑ_{min}	ϑ_{max}
Ti_2SiB	This study	214.11	261.87	2.26	2.52	87.62	119.63	0.07	0.29
Ti_2AlB	Theory [15]	197.67	252.56	2.17	2.68	1.00	115.10	0.09	0.30

5. Vibrational and Thermal Properties

The dynamical stability of *Ti_2SiB* is calculated using finite displacement method in the Phonopy code for a 2x2x1 supercell. The force constants and phonon dispersion frequencies are obtained. The phonon dispersion curve is shown in Figure 6 with partial density of states. *Ti_2SiB* is a dynamically stable material which has only real phonon branches. There are 24 branches where three of them is acoustic and remaining of them

are optical. For these branches, *Ti* atoms contribute at the lower frequencies and *B* atoms contribute higher frequencies as can be seen in Figure 6.

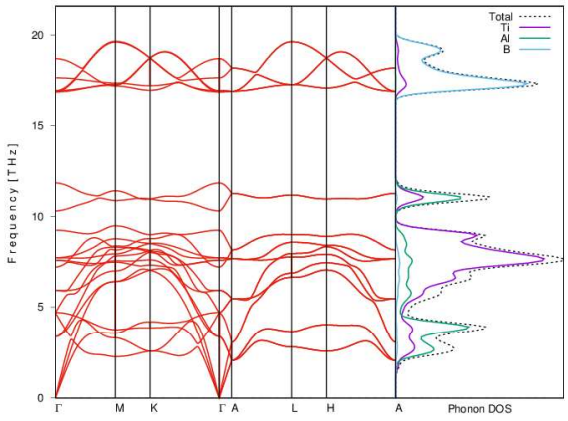

Figure 6. Phonon band structure and partial density of states for Ti_2SiB

Additionally, the phonon frequencies at Γ point for *Ti_2SiB* have been listed in Table 6. The classification of the phonon modes for this material can be given as; $A_{1g}+3A_{2u}+2B_{1g}+2B_{2u}+2E_{2u}+2E_{2g}+3E_{1u}+E_{1g}$.

Table 6: The calculated phonon frequencies (THz) at Γ point of Ti_2SiB.

Symmetry	
E_{1u}	0.001
A_{2u}	0.002
E_{2u}	3.364
B_{2u}	4.674
E_{2g}	4.704
E_{1u}	5.927
B_{1g}	7.216
E_{1g}	7.588
E_{2g}	7.729
A_{1g}	9.254
A_{2u}	10.312
B_{1g}	11.874
E_{2u}	16.861

E_{1u}	16.929
A_{2u}	17.629
B_{2u}	18.687

Here, A_{2u}+E_{1u} belongs to acoustic phonon modes and the others belong to varied optic phonon modes. These optic modes are Raman Active Modes ($\Gamma_R = A_{1g}+E_{1g}+2E_{2g}$), Hyper Raman Active Modes ($\Gamma_H = 2B_{1g}+2B_{2u}+2E_{2u}$) and Infrared Active Modes ($\Gamma_I = 2A_{2u} + 2E_{1u}$). Phonon frequencies of these compounds at Γ point can provide useful information for future experiments to identify the predicted new phases.

The thermal properties are calculated after phonon calculations. Figure 7 shows the entropy, free energy and enthalpy as a function of temperature. The entropy increases while the free energy decreases as the temperature goes from 0 to 2000 K as can be seen from Figure 7. The enthalpy also increases linearly with the temperature after 300 K as can be seen from Figure 7. Figure 8 shows the heat capacity as a function of temperature. It is realized from the figure that when T < 750 K, the Cv increases very rapidly with the temperature; when T > 750 K, the Cv increases slowly with the temperature, and it almost approaches a constant value called as Dulong–Petit limit for this compound.

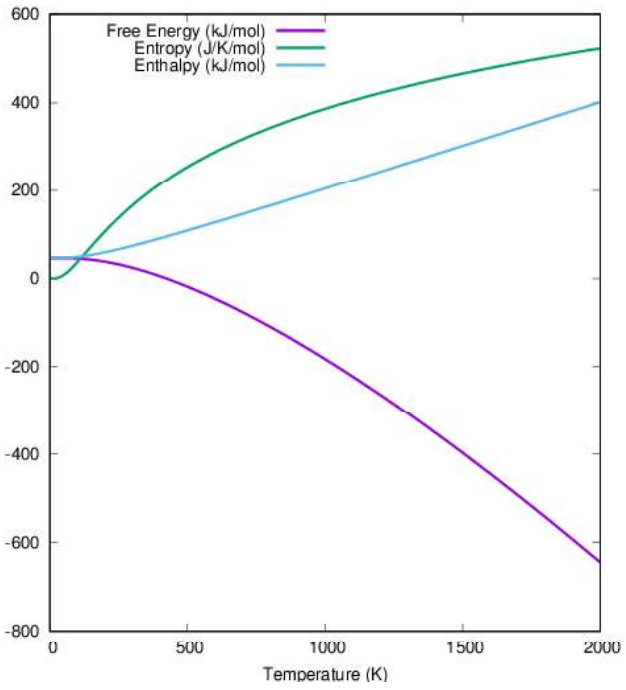

Figure 7. Entropy, free energy and enthalpy as a function of temperature for Ti_2SiB

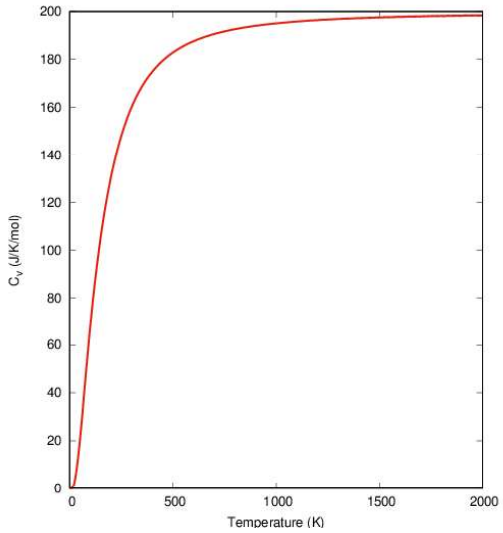

Figure 8. Heat capacity as a function of temperature for Ti_2SiB

6. Conclusion

The structural, mechanic, electronic, and dynamic properties of *Ti_2SiB* have been calculated using VASP. The formation enthalpy of *Ti_2SiB* indicates that this compound is energetically stable and therefore could be synthesized. The band structure shows that *Ti_2SiB* has a metallic character. Moreover, the charge density illustrates that *Ti_2SiB* has dominantly ionic bonding. The calculated elastic constants showed that this compound is mechanically stable. In the calculated phonon dispersion curves, there are no soft modes at any wave vectors, which confirms the dynamical stability of *Ti_2SiB*.

Furthermore, the Raman frequencies are obtained in order to offer practical information for the future experiments. The study has been completed with the investigation of thermodynamic properties of *Ti_2SiB*. Consequently, in this study, *Ti_2SiB* compound, a hypothetical MAX phase, has been investigated and due to its B atom, it is a possible candidate material for the nuclear applications. This is the first study of *Ti_2SiB* as best of our knowledge that could provide insights for both theoretical and experimental studies.

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