Chemically stable new MAX phase $V_2SnC$: a damage and radiation tolerant TBC material

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Using density functional theory, the phase stability and physical properties, including structural, electronic, mechanical, thermal and vibrational with defect processes, of a newly synthesized 211 MAX phase $V_2SnC$ are investigated for the first time. The obtained results are compared with those found in the literature for other existing $M_2SnC$ ($M=Ti, Zr, Hf, Nb$ and $Lu$) phases. The formation of $V_2SnC$ is exothermic and this compound is intrinsically stable in agreement with the experiment. $V_2SnC$ has potential to be etched into 2D MXene. The new phase $V_2SnC$ and existing phase $Nb_2SnC$ are damage tolerant. $V_2SnC$ is elastically more anisotropic than $Ti_2SnC$ and less than the other $M_2SnC$ phases. The electronic band structure and Fermi surface of $V_2SnC$ indicate the possibility of occurrence of its superconductivity. $V_2SnC$ is expected to be a promising TBC material like $Lu_2SnC$. The radiation tolerance in $V_2SnC$ is better than that in $Lu_2SnC$.

1. Introduction

MAX phases are a family of more than 80 ternary carbides, nitrides and borides in hexagonal crystal symmetry. This family is chemically represented as $M_{n+1}AX_n$, where $M$ is an early transition metal, $A$ is an A-group element, $X$ is C or N or B, and the integer ‘$n$’ ranges from 1 to 3. Depending on the value of layer index $n$, MAX phases are categorized as 211, 312 and 413 phases for $n = 1, 2, 3$, respectively. MAX phases crystallize in the hexagonal space group $P6_3/mmc$ (194). In their crystal structures, $M_nX$-octahedra with the $X$-elements fill the octahedral positions between the $M$-elements as do in the corresponding MX binaries. The octahedra exchange with the $A$-atomic layers placed at the centers of trigonal prisms, which are larger, and thus more accommodating of the larger $A$-atoms. The interposing pure metallic $A$-atomic planes are mirror planes to the meandering ceramic $M_nX_n$ slabs. Due to alternating metallic and ceramic layers in MAX phases they possess a unique set of metallic and ceramic properties. The common metallic properties are electrical and thermal conductivities, high fracture toughness, machinability, damage tolerant and thermal shock resistance. The typical ceramic properties are lightweight, oxidation and corrosion resistance, elastic stiffness, resistant to fatigue and ability to maintain the strength to high temperature. The MAX phases also experience plastic-to-brittle transitions at high temperatures, and can resist high compressive stresses at ambient temperature. These exceptional properties of MAX phases make them suitable for potential uses as tough and machinable, coatings for electrical contacts, thermal shock refractories, and heating elements at high temperature. Additionally, their neutron irradiation resistance makes them suitable in nuclear applications. A common recent use of MAX phases is as precursors for producing two-dimensional MXenes. The MAX phases are attractive due to their unique combination of structural characteristics, wide range of properties, and many prospective uses.

Early studies on $M_2SnC$ phases by Jeitschko et al. in mid 1960s resulted in synthesized phases with $M=Ti, Zr, Hf, and Nb$. Kuchida et al. synthesized the first Lu-based MAX phase $Lu_2SnC$ in the $M_2SnC$ family. Lu is the last element in the lanthanide series although it sometimes mentioned as the first member in the 6th-period transition metals. Lu replaced the common early transition metals “$M$” in the $M_2SnC$ MAX phases. Theoretical investigations reveal that $Lu_2SnC$ is softer and more easily machinable than the other existing $M_2SnC$ phases. It is also a promising candidate as a thermal barrier coating (TBC) material owing to its high thermal shock resistance, low minimum thermal conductivity, high melting temperature and characteristically good oxidation resistance. Xu et al. focused their attention on $M_2SnC$ phases and synthesized $V_2SnC$ by sintering $V$, $Sn$, and $C$ powder mixture at $1000^\circ C$. They identified the crystal structure of $V_2SnC$ as 211 MAX phases through X-ray diffraction, first-principles calculation, and high-resolution transmission scanning electron microscopy.
M$_2$SnC compounds show diversity in their properties. Nb$_2$SnC and Lu$_2$SnC show superconducting transition, Nb$_2$SnC has also better radiation tolerance in the M$_2$SnC family, Hf$_2$SnC is highly dense, and Zr$_2$SnC is highly elastically anisotropic in this group. Additionally, the lattice constants of Sn-containing 211 MAX phases show an increasing trend with the crystal radius of M-elements. The diverse properties of M$_2$SnC motivated the use of density functional theory (DFT) calculations to explore the physical properties of V$_2$SnC and the analysis of the trend of physical properties in M$_2$SnC MAX phases. In this study, the mechanical, lattice dynamical and thermodynamic phase stability is examined for the new phase V$_2$SnC. Mechanical behaviors, elastic anisotropy, Debye temperature, melting point, lattice thermal conductivity, minimum thermal conductivity, lattice dynamics and defect processes of V$_2$SnC are investigated for the first time.

2. Methodology

All calculations are performed with the DFT method as implemented in CASTEP. The non-spin polarized Perdew–Burke–Ernzerhof (PBE) functional within generalized gradient approximation (GGA) is chosen to describe the electronic exchange-correlation potential. Ultra-soft pseudo-potential developed by Vanderbilt is used to model the interactions between electrons and ion cores. A Γ-centered k-point mesh of $15 \times 15 \times 3$ grid in the Monkhorst-Pack (MP) scheme is used to integrate over the first Brillouin zone in the reciprocal space of the MAX phase hexagonal unit cell. To expand the eigenfunctions of the valence and closely valence electrons in terms of a plane-wave basis, a cutoff energy of 700 eV is chosen. Total energy and internal forces are minimized during the geometry optimization with the BFGS minimization technique named this method implemented in the CASTEP code. The self-consistence convergence is achieved with the difference in the total energy within $5 \times 10^{-6}$ eV per atom, the maximum ionic Hellmann–Feynman force within 0.01 eV Å$^{-1}$, maximum ionic displacement within $5 \times 10^{-4}$ Å, and maximum stress within 0.02 GPa. For self-consistent field calculations, the tolerance is chosen as $5 \times 10^{-7}$ eV per atom.

The elastic stiffness constants and moduli are calculated from the first-principles investigations using finite-strain method implemented in the CASTEP code. This method involves setting the deformation to a predetermined value, relaxing all free parameters and computing the stress. The convergence criteria for elastic calculations are chosen as: the difference in total energy within $10^{-6}$ eV per atom, the maximum ionic Hellmann–Feynman force within $2 \times 10^{-3}$ eV Å$^{-1}$, and the maximum ionic displacement within $10^{-4}$ Å. Elastic calculations with CASEP code have been successful for all kind of crystal systems. The lattice dynamic properties such as phonon dispersion and phonon density of states are calculated by means of the finite displacement supercell method executed with a $3 \times 3 \times 1$ supercell within the code.

Defect calculations are performed with a 72-atomic site (36M, 18A, and 18C) supercell using a $3 \times 3 \times 1$ MP k-point mesh under constant pressure. Allowing for all possible interstitial sites, an intensive computational search is carried out to identify the potential interstitial sites. The defect energies are defined as effectively energy differences between the isolated defects.

3. Results and discussion

3.1. Structural aspects and phase stability

The newly synthesized V$_2$SnC phase crystalizes in the hexagonal MAX phase crystal structure with space group P6$_3$/mmc (no. 194). The position of each atom is found as V at 4f ($1/3, 2/3, 0.0744$), Sn at 2d ($2/3, 1/3, 1/4$), and C at 2a (0, 0, 0). The V and Sn atoms stack along the z-direction (c-axis) (see Fig. 1, where M represents V, A refers to Sn and X is C). There are two layers of V atoms in each V–C slab, and every two layers of V atoms and one layer of Sn atoms are consecutively arranged along the z-direction. The optimized lattice constants $a$ and $c$ and internal parameter $z_M$ are in agreement with the experimental and theoretical values. The present values ($a = 3.121$ Å, $c = 12.947$ Å, $z_M = 0.0759$) are closer to the experimental results ($a = 2.981$ Å, $c = 13.470$ Å, $z_M = 0.0776$) compared with the previous theoretical values ($a = 3.134$ Å, $c = 12.943$ Å, $z_M = 0.0751$). The reason may be the use of coarse k-point mesh ($9 \times 9 \times 2$) and low cutoff energy (400 eV) in the previous theoretical study. In the M$_2$SnC systems, we observed that the unit cell parameters show a better relationship with the crystal radius of M atoms. In this relation, the lattice parameters exhibit increasing trend with the increase of crystal radius of transition metal M. The newly synthesized V$_2$SnC also obeys this relation (refer to Fig. 2) (Table 1).

Phase stability of MAX phases with respect to the constituent elements cannot be used to predict whether a material is thermodynamically stable. Instead, all competing phases need to be included in the analysis. The thermodynamic stability of the recently synthesized V$_2$SnC MAX phase is examined at 0 K with respect to decomposition into any combination of competing phases. The most competitive set of competing phases, designated as equilibrium simplex, is identified using a linear optimization procedure. This procedure has already been

![Fig. 1](image-url) (a) Crystal structure and (b) 2D view in yz-plane of 211 MAX phase.
Elastic constants also provide a fundamental insight into the nature of bonding character between adjacent atomic planes and the anisotropic character of the bonding and structural stability. They can link between a material’s dynamical behaviour and its mechanical and thermal properties. For hexagonal MAX phases, five nonzero independent elastic constants, namely $C_{11}$, $C_{12}$, $C_{13}$, $C_{33}$, and $C_{44}$ are obtained.14 Table 3 lists the elastic constants of the newly synthesized $V_2SnC$ calculated at zero pressure and zero temperature along with the values found in literatures for existing $M_2SnC$ phases for comparison. For $Ti_2SnC$, $Nb_2SnC$, $Hf_2SnC$, and $Zr_2SnC$, we have listed $C_{ij}$ calculated with either different codes or different functionals. The CASTEP-GGA results are consistent to the VASP-GGA values.

Elastic constants are listed in Table 2. The elastic constants of $M_2SnC$ phases, including newly synthesized $V_2SnC$, are calculated with CASTEP-GGA, in which the bond-order and its mechanical and thermal properties. For hexagonal $\text{MAX phases}$, five nonzero independent elastic constants, namely $C_{11}$, $C_{12}$, $C_{13}$, $C_{33}$, and $C_{44}$ are obtained.14 Table 3 lists the elastic constants of the newly synthesized $V_2SnC$ calculated at zero pressure and zero temperature along with the values found in literatures for existing $M_2SnC$ phases for comparison. For $Ti_2SnC$, $Nb_2SnC$, $Hf_2SnC$, and $Zr_2SnC$, we have listed $C_{ij}$ calculated with either different codes or different functionals. The CASTEP-GGA results are consistent to the VASP-GGA values.

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is applied along the $a$-axis. The phase Nb$_2$SnC is most capable to resist such deformation, while Lu$_2$SnC will deform easily under the same stress along the $a$-axis. The new compound V$_2$SnC is the next most capable phase to resist the deformation in M$_2$SnC systems if a rank is made one obtains: Nb$_2$SnC > V$_2$SnC > Hf$_2$SnC > Ti$_2$SnC > Zr$_2$SnC > Lu$_2$SnC.

### Table 3 Elastic properties of M$_2$SnC (M = V, Ti, Zr, Nb and Hf) MAX phases

| Phases | $C_{11}$ | $C_{12}$ | $C_{44}$ | $C_{66}$ | $B$ | $G$ | $E$ (eV fu$^{-1}$) | $v$ | $B/G$ | Remarks |
|--------|----------|----------|----------|----------|-----|----|-----------------|-----|------|---------|
| V$_2$SnC | 243      | 300      | 87       | 84       | 76  | 124 | 156             | 82  | 0.276 | 1.91 CASTEP-GGA (This work) |
| Lu$_2$SnC | 336      | 304      | 85       | 105      | 122 | 122 | 190             | 81  | 0.199 | 1.33 CASTEP-GGA$^{12}$ |
| Ti$_2$SnC | 172      | 173      | 56       | 64       | 46  | 36  | 82              | 61  | 0.197 | 1.27 FP-L/APW + lo$^{57}$ |
| Zr$_2$SnC | 268      | 265      | 100      | 95       | 79  | 74  | 139             | 97  | 0.217 | 1.43 CASTEP-GGA$^{12}$ |
| Hf$_2$SnC | 253      | 254      | 93       | 79       | 91  | 74  | 138             | 87  | 0.218 | 1.37 FP-L/APW + lo$^{57}$ |
| Nb$_2$SnC | 303      | 308      | 121      | 109      | 84  | 88  | 160             | 114 | 0.212 | 1.40 CASTEP-LDA$^{48}$ |

**Table 2** Lattice parameters, unit cell volume and total energies of V$_2$SnC and its competing phases

| Phase | Prototype structure | Pearson symbol | Space group | $a$ (Å) | $b$ (Å) | $c$ (Å) | $V$ (Å$^3$) | $E$ (eV/atom) |
|-------|---------------------|----------------|-------------|--------|--------|--------|------------|--------------|
| C     | C (graphite)        | hP4            | P6$_3$/mmc  | 194    | 2.462744 | 2.462744 | 8.985673  | 47.2        |
| V     | W                   | c12            | I3m (229)   | 3.011843 | 3.011843 | 3.011843 | 9.035481  | 27.3        |
| V-Sn | Diamond             | fF8            | Fd3m (227)  | 3.567776 | 3.567776 | 3.567776 | 11.72330  | 54.4        |
| V-Sn | Inverse CdI$_2$     | hP3            | P6$_3$/mmc  | 194    | 3.084133 | 3.084133 | 3.084133 | 9.242403   |

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We have obtained the bulk modulus $B$ and shear modulus $G$ of polycrystalline aggregates from individual elastic constants, $C_{ij}$ by the Hill approximations as implemented within the code.\(^{38}\) Using $B$ and $G$, the average Young’s modulus $E$ and the Poisson ratio $\nu$ can be obtained:

$$E = \frac{9BG}{3B + G}$$  \hspace{1cm} (4)

and

$$\nu = \frac{3B - 2G}{6B + 2G}$$  \hspace{1cm} (5)

All the elastic moduli $B$, $G$, and $E$ and Poisson’s ratio $\nu$ are also listed in Table 3, from which we observe that the results obtained with the CASTEP-GGA and VASP-GGA are consistent to each other, while the other results deviate considerably. Fig. 3b presents elastic moduli calculated with the CASTEP-GGA scheme. $B$ is highly correlated to the chemical composition and structure, while $G$ is linked to chemical bonding. On the other hand, $E$ measures the response under uniaxial tension averaged over all directions. Within the results of this scheme, $B$ is highest for Nb$_2$SnC (160 GPa) and lowest for Lu$_2$SnC (82 GPa). The new phase V$_2$SnC has second highest value of 156 GPa. Ti$_2$SnC has highest $G$ (97 GPa) and $E$ (236 GPa) values. The lowest values of $G$ (61 GPa) and $E$ (147 GPa) are found for Lu$_2$SnC. The new phase V$_2$SnC has an intermediate value of $G$ (80 GPa) and $E$ (209 GPa). When we move from left to right in the Fig. 3b, we cross the group-3 element (Lu) to group-5 elements (V, Nb) via the group-4 elements (Ti, Zr, Hf). The elastic moduli $G$ and $E$ show the almost similar trend. $B$ of the phases containing groups 3 and 4 elements as M-atom show the similar trend of $G$ and $E$ but the phases containing the group-5 elements show the reverse trend. For comparison, we have found $152 \pm 3$, $180 \pm 5$, and $169 \pm 4$ GPa as the measured values of $B$ for Ti$_2$SnC, Nb$_2$SnC, and Hf$_2$SnC, respectively.\(^{39,40}\) These values are larger than the values calculated with GGA within CASTEP and VASP codes by $9$–$14\%$ and smaller than the other values by $2$–$16\%$. The experimental shear modulus is found for Ti$_2$SnC, which is comparable with the GGA-value and much smaller than the other theoretical values listed in Table 3.\(^{41}\) The experimental Poisson’s ratio for Ti$_2$SnC is $0.24$, which is also very close to the GGA-values rather than other values.\(^{41}\) The experimental value of $E$ for Ti$_2$SnC, Nb$_2$SnC, Zr$_2$SnC, and Hf$_2$SnC are $207.4$, $216$, $178$, and $237$ GPa, respectively.\(^{40,41}\) For Nb$_2$SnC and Hf$_2$SnC, the experimental $E$ is larger than the theoretical $E$ calculated with both the CASTEP-GGA and VASP-GGA by $7$–$8\%$, while the experiment $E$ of Ti$_2$SnC and Zr$_2$SnC is smaller than the theoretical $E$ derived with GGA within CASTEP and VASP codes by $5$–$16\%$. From other theoretical values listed in Table 3, the experimental $E$ deviates within $13$–$51\%$. Therefore, the GGA values of $B$ and $E$ obtained with the CASTEP and VASP codes deviates from experimental values within a reasonable range. The larger the $E$ value, the stiffer the system, and therefore the larger the exfoliation energy.\(^{42}\) Amongst the productively etched MAX phases into two-dimensional (2D) MXenes, V$_2$AlC has the largest theoretical exfoliation energy, whose $E$ is reported $311$ and $316$ GPa.\(^{43,44}\) Accordingly, the exfoliation energy of new MAX phase V$_2$SnC and previously observed M$_2$SnC have lower exfoliation energy than V$_2$AlC. It is evident that all M$_2$SnC (M = V, Ti, Zr, Hf, Nb, and Lu) phases have potential to etch into 2D MXenes.

Poisson’s ratio $\nu$ provides the information regarding the bonding forces and reflects the stability of a material against shear. The M$_2$SnC MAX phases including newly synthesized V$_2$SnC have Poisson’s ratio within $0.195$–$0.290$. As the obtained values with CASTEP-GGA for V$_2$SnC, Hf$_2$SnC and Nb$_2$SnC fall in the range of $0.25$–$0.3$; their interatomic forces can be considered as central forces.\(^{45}\) Literature values of $\nu$ for Hf$_2$SnC\(^{46,48}\) lie on the lower side of this range, while a literature value for Zr$_2$SnC\(^{46}\) falls within this range. The values outside this range indicate that the interatomic force is non-central. The low value of $\nu$ for Lu$_2$SnC indicates that it is more stable against shear than other M$_2$SnC phases including the new phase V$_2$SnC.\(^{1}\) Additionally, a pure covalent crystal has a Poisson’s ratio of $0.1$ and a totally metallic compound has a value of $0.33$. As the Poisson’s ratio for M$_2$SnC MAX phases lies between these two characteristic values their atomic bonding is expected to be a mixture of covalent and metallic in nature. Furthermore, Poisson’s ratio can classify the solid materials as either brittle or ductile with a value of $0.26$.\(^{49,50}\) Brittle materials have values less than $0.26$ and ductile materials have values larger than this value. Accordingly, the new phase V$_2$SnC and Nb$_2$SnC are ductile and the remaining phases are brittle. Therefore, V$_2$SnC and Nb$_2$SnC are predicted to be damage tolerant.

Bulk modulus to shear modulus ratio ($B/G$), known as Pugh’s ratio can serve as a tool for measuring the ductile/brittle nature
If the Pugh's ratio is greater than 1.75 the material is expected to be ductile, otherwise it is brittle in nature. Accordingly, V$_2$SnC and Nb$_2$SnC are ductile in nature as predicted from their Poisson's ratio.

Indeed, it is essential to analyze and visualize the directional dependence of elastic properties – such as Young's modulus ($E$), linear compressibility ($\beta$), shear modulus ($G$) and Poisson's ratio ($\nu$) of anisotropic materials – rather than their averages.
For the M₂SnC phases, the directional dependency of $E$, $\beta$, $G$ and $\nu$ are calculated using the ELATE suit program and the 2D presentations are shown in Fig. 4 for V₂SnC, indicating that there is no directional dependence in the $xy$ plane as the plots are uniformly circular but in both $xz$ and $yz$ planes there are directional dependences and which are similar in nature as the hexagonal crystal symmetry of V₂SnC. The linear compressibility for some compounds can be negative in some directions, which is represented with an additional curve of red color. For V₂SnC, no negative value is found for any direction. The shear modulus $G$ and Poisson’s ratio $\nu$ are not so straightforward to represent, as they depend on two orthogonal unit vectors $a$ and $b$, which respectively represent the direction of the stress applied and the direction of measurement. For $G$ and $\nu$ there are two curves: translucent blue curve represents the maximal values and green curve represents the minimal positive values. There are a lot of compounds having negative Poisson’s ratio in some directions. In this case, an additional curve of translucent red represents the negative values. For V₂SnC, no negative Poisson’s ratio is found for any direction. The shear anisotropy in the {001} shear planes between the $h0i$ and $h01$ directions; and

$$\text{elastic anisotropy } A_x = \left\{ \begin{array}{ll} \frac{X_{\text{max}}}{X_{\text{min}}} & \text{if } \text{sign}(X_{\text{max}}) = \text{sign}(X_{\text{min}}) \\ \text{otherwise} & \end{array} \right.$$  (6)

The obtained elastic anisotropy $A_x$ for each elastic modulus is also listed in Table 4. It is observed that Young’s modulus shows maximum anisotropy for Nb₂SnC and minimum for Ti₂SnC. Anisotropy in linear compressibility is maximum for V₂SnC and minimum for Ti₂SnC. Anisotropy in shear modulus is highest for Hf₂SnC and lowest for Ti₂SnC. Maximum anisotropy of Poisson’s ratio is observed in Hf₂SnC and minimum in Ti₂SnC. Considering all parameters Ti₂SnC is the least anisotropic in M₂SnC family.

Here, we want to quantify the degree of elastic anisotropy of V₂SnC and compare with previously synthesized M₂SnC phases. For hexagonal M₂SnC crystals, there are three shear anisotropy factors linked to $C_{ij}$ that can be determined using the succeeding expressions:

$$A_1 = \frac{(C_{11} + C_{12} + 2C_{33})}{6C_{44}},$$  (7)

which is associated with the {010} shear planes between the $\langle 011 \rangle$ and $\langle 010 \rangle$ directions;

$$A_2 = \frac{2C_{44}}{C_{11} - C_{12}},$$  (8)

which is related to the {010} shear planes between the $\langle 101 \rangle$ and $\langle 001 \rangle$ directions; and finally,

$$A_3 = \frac{(C_{11} + C_{12} + 2C_{33} - 4C_{13})}{3(C_{11} - C_{12})},$$  (9)

which signifies shear anisotropy in the {001} shear planes between the $\langle 110 \rangle$ and $\langle 010 \rangle$ directions. For isotropic crystals,

Table 4 Minimal and maximal values of each modulus and elastic anisotropy obtained from them

| Phases | Young’s modulus (GPa) | Linear compressibility (TPa⁻¹) | Shear modulus (GPa) | Poisson’s ratio |
|--------|-----------------------|-------------------------------|---------------------|----------------|
| V₂SnC  | 188.79                | 1.0964 2.7112                | 71.355 86.673      | 0.12849 0.38828 |
| Hf₂SnC | 168.97                | 1.9579 2.4831                | 66.846 99.802      | 0.12198 0.38969 |
| Lu₂SnC | 143.59                | 3.8307 3.9590                | 56.841 70.092      | 0.16641 0.26442 |
| Nb₂SnC | 168.47                | 1.7785 2.1490                | 66.303 97.202      | 0.15262 0.41665 |
| Ti₂SnC | 233.72                | 2.4154 2.4509                | 95.408 100.210     | 0.19446 0.22531 |
| Zr₂SnC | 174.63                | 2.1404 2.7889                | 68.418 94.736      | 0.13615 0.33803 |

Elastic anisotropy $A_x$

| $A_x$  | $A_y$  | $A_c$  | $A_v$  |
|--------|--------|--------|--------|
| V₂SnC  | 1.186  | 2.4729 | 1.215  | 3.0219 |
| Hf₂SnC | 1.399  | 2.674  | 1.493  | 3.1947 |
| Lu₂SnC | 1.166  | 1.0335 | 1.233  | 1.5889 |
| Nb₂SnC | 1.408  | 1.2083 | 1.466  | 2.7300 |
| Ti₂SnC | 1.024  | 1.0147 | 1.050  | 1.1586 |
| Zr₂SnC | 1.276  | 1.3030 | 1.385  | 2.4828 |
all $A_i$’s ($i = 1, 2, 3$) have unit value. A value other than unity quantifies the anisotropic state of crystals. The deviation of $A_i$ from unity ($\Delta A_i$) measures the level of elastic anisotropy in shear.

The calculated values of $A_i$ for V$_2$SnC are listed in Table 5 along with reported values for other M$_2$SnC phases and the anisotropy level $\Delta A_i$ is shown in Fig. 5, suggesting that all M$_2$SnC phases including V$_2$SnC are elastically anisotropic in shear. Shear anisotropy level is highest in Nb$_2$SnC and lowest in Ti$_2$SnC in all respects. The anisotropy level in the new phase V$_2$SnC is higher than that in Ti$_2$SnC and lower than those in other M$_2$SnC phases. It is observed that the shear anisotropy level within a group of M atoms of M$_2$SnC phases increases in the descending order. A different anisotropy factor for hexagonal crystals depending on $C_{ij}$, i.e., $k_c/k_a = (C_{11} + C_{12} - 2C_{13})/(C_{13} - C_{11})$ is used to quantify the elastic anisotropy upon compression; where $k_a$ and $k_c$ are the linear compressibility coefficients along the $a$- and $c$-axis, respectively.\(^{34}\) Deviation of $k_c/k_a$ from unity ($\Delta(k_c/k_a)$), determines the anisotropy level upon linear compression. The calculated value reveals that the compressibility along the $c$-axis is smaller than that along the $a$-axis for the new phase V$_2$SnC as well as for Zr$_2$SnC, Hf$_2$SnC, and Nb$_2$SnC. For Lu$_2$SnC and Ti$_2$SnC the compressibility along the $c$-axis is greater than that along the $a$-axis.

According to Hill, the difference between $B_c$ and $B_R$ as well as $G_V$ and $G_R$ is proportional to the degree of elastic anisotropy of crystals, which leads to define the percentage anisotropy factors $A_B$ and $A_G$ with the succeeding equations:\(^{35}\)

$$A_B = \frac{B_c - B_R}{B_V + B_R} \times 100\%$$

The percentage anisotropy factors $A_B$ and $A_G$ calculated for V$_2$SnC are also listed in Table 5 together with the literature value of other M$_2$SnC phases. These two factors assign zero values for completely isotropic crystals in view of compressibility and shear, respectively. A positive value quantifies the level of anisotropy. It is evident that the new phase V$_2$SnC is more anisotropic in compression, whereas Nb$_2$SnC is more anisotropic in shear. Nb$_2$SnC is less anisotropic in compression and Ti$_2$SnC is less anisotropic in shear. An anisotropy factor named “universal anisotropy index” is recently proposed for an appropriate universal measure of elastic anisotropy of crystals and defined as:\(^{36}\)

$$A_U = \frac{G_V - G_R}{G_V + G_R} \times 100\%$$

This index has either zero or positive value. Zero value signifies the completely isotropic nature and positive value indicates the anisotropy level in elastic properties of crystals. According to this index (see Table 5), the new phase V$_2$SnC is more anisotropic than Lu$_2$SnC, Ti$_2$SnC and Zr$_2$SnC and less anisotropic than Hf$_2$SnC and Nb$_2$SnC. It is evident that the universal anisotropy level follows the trend of shear anisotropy level. That is, the universal anisotropy level within a group of M atoms of M$_2$SnC phases increases in the descending order.

### 3.3. Electronic properties

Electronic structure plays a significant role in understanding of material properties at the microscopic level. Electronic energy band structure calculated along high symmetry points of the Brillouin zone for V$_2$SnC is shown in Fig. 6a. Similar to other M$_2$SnC and remaining MAX phases, the band structure of V$_2$SnC reveals the metallic characteristics as a large number of its valence bands cross the Fermi level $E_F$ and overlap with the conduction bands. The position of Fermi level in V$_2$SnC is just below the valence band maximum near the $\Gamma$-point as in the band structure of V$_2$SnC is very similar to that of...
Weaker M than V states per eV per unit cell. This arises due to Sn-s orbitals in similar to in other M2SnC and two main parts. An intermediate low MAX phases.

The Fermi level of V2SnC lies far from a pseudogap at the left and C-2s states, which indicate strong covalent V-Sn bonds, respectively. Analogous bonds are also seen in the contour maps of other M2SnC compounds. The spherical charge distributions around the atoms also indicate some ionic nature in chemical bonds in V2SnC as well as in other M2SnC MAX phases.

The Fermi surface (FS) calculated for the V2SnC MAX phase is shown in Fig. 7b, which contains four different sheets. All sheets are seen to be centered along the Γ-A direction. The first and second sheets are cylindrical. They have an extra part like a half-folded plain sheet along each L-M direction. The third sheet shows a lot of nesting nature. It has also an additional

Fig. 6 Electronic structures of V2SnC, (a) band structure and (b) density of states; $E_F$ denotes the Fermi level.

We have calculated the electron charge density map and Fermi surface to understand the nature of chemical bonding in V2SnC. In the contour map of electron charge density (Fig. 7a) it is seen that the charge distributions around V atoms are practically spherical and its intensity specifies the amount of charge accumulation. The charge accumulated around the V atom is 0.32e, whereas the charge accumulation around the M atoms in other M2SnC systems ranges from 0.28-0.45e. The highest charge is deposited around the Lu atom (0.45e) and lowest charge around the Hf atom (028e). The V-charge overlaps with the C-charge and slightly edges with the Sn-charge, which indicates the strong V-C and weak V-Sn bonds, respectively.

The overall bonding nature in the new phase V2SnC as well as in other M2SnC MAX phases.

Fig. 7 Electronic structures of V2SnC; (a) charge density map, (b) Fermi surface and (c) fourth Fermi sheet.

Sn2SnC rather than other M2SnC phases. Nb2SnC is a superconducting phase. Resemblance of two band structures indicates the possibility of superconductivity in V2SnC. The main characteristic of the band structure is the significantly anisotropic nature with less energy dispersion along the c-axis. It is evident from the reduced dispersion along the short H-K and M-L directions. The anisotropic band structure near and below the Fermi level implies that the electrical conductivity is also anisotropic for the new MAX phase studied here.

To realize the bonding nature, the total and partial density of states (DOS) are calculated for V2SnC and presented in Fig. 6b. The Fermi level of V2SnC lies far from a pseudogap at the left and instead of near a pseudogap as found for other existing M2SnC MAX phases. Consequently, the new phase V2SnC is not as stable as other M2SnC phases. In fact, the Fermi level of V2SnC lies at the wall of a large peak and as a result V2SnC has a large total DOS of 6.12 states per eV per unit cell at $E_F$, whereas the total DOS at $E_F$ for other M2SnC phases ranges from 2.35–3.93 states per eV per unit cell. The valence band of V2SnC contains two main parts. An intermediate low flat-type valence band arises due to Sn-s orbitals in similar to in other M2SnC and M2SnC2 compounds.

The lower valence band consists of a single peak arising owing to the hybridization between V-3d and C-2s states, which indicate strong covalent V-C bond in V2SnC similar to the M-C bonds in M2SnC. The higher valence band contains three distinct peaks similar to those of Nb2SnC. The small peak at the left of the higher valence band arises due to the interaction between V-3d and C-2p-orbitals. The middle peak is the highest peak and arises owing to the hybridization between V-3d and C-2p electrons. The third peak corresponds to the interaction between V-3d and Sn-5p states. This interaction results in weaker covalent V-Sn bonding due to closeness of the peak to the Fermi level. It is clear that the V-C bond is stronger than V-Sn bond as M-C bonds are stronger than M-A bonds. Weaker M-A bond favours the exfoliation of M2SnC MAX phases to 2D MXenes. The overall bonding nature in the new phase V2SnC is a combination of metallic, covalent, and, due to the difference in electronegativity between the constituent atoms, ionic like other MAX phase compounds.
part along H–K directions, whose shape is like a cylinder cutting parallel to its axis. The fourth sheet consists of two identical parts along the H–K directions. The lower part is just the mirror inversion of the upper part (Fig. 7c). As seen from Fig. 5a, near the Γ (0,0,0) point, two hole-like bands appear, giving rise to two hole-like Fermi surface sheets near the Γ point (first and second sheets). Conversely, the calculated band structure near the H(1/3, 1/3, 1/3) point consists of two electron-like bands, corresponding to two electron-like Fermi surface sheets near the H point (third and fourth sheets). The FS of V_2SnC has a lot of similarities to that of superconducting Nb_2SnC among all M_2SnC MAX phases. Nb_2SnC is a superconducting phase having nesting nature in its FS. This nesting plays a role in strong electron–phonon interactions and is ultimately able to enhance the superconducting order of the material. Nesting nature is an indication of superconductivity of V_2SnC. We hope that the experimentalists will be stimulated to confirm the prediction.

3.4. Thermal properties

In this section, we have reported the elastic Debye temperature, melting point, lattice thermal conductivity and minimum thermal conductivity of V_2SnC. Debye temperature \( \theta_D \) is a characteristic temperature of solid materials that can be calculated from the elastic moduli using Anderson method. This method is simple and rigorous, which determines \( \theta_D \) using average sound velocity calculated from the shear and bulk moduli via the equation:

\[
\theta_D = \frac{h}{k_B} \left[ \left( \frac{3n}{4\pi^2} \frac{N\alpha^0}{M} \right)^{1/3} T_{\text{m}} \right]^{1/3},
\]

where \( h \) is Planck’s constant, \( k_B \) is Boltzmann constant, \( N \) is Avogadro’s number, \( \alpha^0 \) is the Grüneisen parameter, \( M \) is the molecular weight and \( T_{\text{m}} \) is the melting point. The obtained sound velocities and Debye temperature of V_2SnC is listed in Table 6 along with the literature values for existing M_2SnC phases and the CASTEP-GGA values are given in Fig. 8. There are several sets of literature values of \( \theta_D \) for M = Ti, Zr, Hf, and Nb. It is observed that the values derived with the GGA functional using the CASTEP and VASP codes are consistent as we have a close measured value (380 K) and a theoretical value (412 K) of \( \theta_D \) for Nb_2SnC. The remaining two sets of \( \theta_D \) values show large deviations from the former sets as well as from the available experimental and theoretical values. It is evident from the Fig. 8 that the sound velocities and Debye temperature follow the reverse trend of shear and universal anisotropy level. That is, the sound velocities and Debye temperature within a group of M atoms of M_2SnC phases decrease in the descending order.

In this equation, \( h \) and \( k_B \) are respectively the Plank and Boltzmann constants, \( N_A \) is Avogadro’s number, \( \rho \) is the mass density, \( n \) is the number of atoms in a molecule, and \( M \) is the molecular weight. The average sound velocity \( v_m \) is obtained from the longitudinal and transverse sound velocities \( v_l \) and \( v_t \) by the equation:

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

With the bulk modulus \( B \) and shear modulus \( G \), \( v_l \) and \( v_t \) can be determined as:

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

The obtained sound velocities and Debye temperature of V_2SnC are in Table 6 along with the literature values for existing M_2SnC phases and the CASTEP-GGA values are given in Fig. 8. There are several sets of literature values of \( \theta_D \) for M = Ti, Zr, Hf, and Nb. It is observed that the values derived with the GGA functional using the CASTEP and VASP codes are consistent as we have a close measured value (380 K) and a theoretical value (412 K) of \( \theta_D \) for Nb_2SnC. The remaining two sets of \( \theta_D \) values show large deviations from the former sets as well as from the available experimental and theoretical values. It is evident from the Fig. 8 that the sound velocities and Debye temperature follow the reverse trend of shear and universal anisotropy level. That is, the sound velocities and Debye temperature within a group of M atoms of M_2SnC phases decrease in the descending order.

The Debye temperatures of M_2SnC MAX phases follow the order of Lu_2SnC < Hf_2SnC < Nb_2SnC < Zr_2SnC < V_2SnC < Ti_2SnC. High average sound velocity corresponds to a high Debye temperature.

### Table 6: Sound velocities in km s\(^{-1}\), Debye temperature and melting point in K, minimum and lattice thermal conductivity in W m\(^{-1}\) K\(^{-1}\) of M_2SnC (M = Lu, Ti, Zr, Hf and Nb) MAX phases

| Phases   | \( \rho \) | \( v_l \) | \( v_t \) | \( v_m \) | \( \theta_D \) | \( T_{\text{m}} \) | \( \kappa_{\min} \) | \( \kappa_{\text{ph}} \) | Remarks                |
|----------|------------|----------|----------|----------|-------------|-------------|----------------|----------------|------------------------|
| V_2SnC   | 7.073      | 6.125    | 3.405    | 3.792    | 472         | 1533        | 1.20           | 14.38          | CASTEP-GGA (This work)|
| Lu_2SnC  | 9.847      | 4.073    | 2.489    | 2.748    | 300         | 1130        | 0.51           | 14.91          | CASTEP-GGA           |
| Ti_2SnC  | 6.346      | 6.503    | 3.910    | 4.325    | 525         | 1556        | 0.99           | 29.98          | CASTEP-GGA           |
| Zr_2SnC  | 7.313      | 7.113    | 4.337    | 4.790    | 561         | 1725        | 1.08           | 36.87          | CASTEP-LDA           |
| Hf_2SnC  | 11.796     | 4.695    | 2.716    | 3.446    | 398         | 1782        | 0.72           | 22.24          | VASP-GGA             |
| Nb_2SnC  | 8.389      | 6.358    | 3.626    | 4.030    | 480         | 1859        | 0.89           | 29.96          | CASTEP-GGA           |
|          | 8.53       | 6.150    | 3.493    | 3.883    | 469         | 1763        | 0.87           | 22.92          | CASTEP-LDA           |

\( ^a \) Calculated from published data. \( ^b \) Calculated at 300 K.
temperature of Ti₂SnC. The new phase V₂SnC has the second highest Debye temperature. Lu₂SnC has a low Debye temperature because of its low average sound velocity. Generally, the higher the Debye temperature the stiffer the material. Therefore, V₂SnC is softer than Ti₂SnC and stiffer than the other existing M₂SnC MAX phases. A low Debye temperature results in low thermal conductivity of a material, which favors it for being a promising thermal barrier coating (TBC) material. The Debye temperature of a promising TBC material, Y₄Al₂O₉ is 564 K, which is larger than those of existing M₂SnC phases. Therefore, M₂SnC phases including new phase V₂SnC have possibility to be potential TBC materials if they have low thermal conductivity, high thermal expansion coefficient, high melting point and oxidation resistance. For comparison, we have experimental Debye temperature only for Nb₂SnC (380 K), which is comparable to the theoretical value (412 K).

Lattice thermal conductivity is one of the most fundamental properties of solids. As the MAX phases have dual characters of metals and ceramics, therefore, to determine their lattice thermal conductivity, the Slack model is appropriate as it deals with materials having partial ceramic nature. The model considers the average of the atoms \( \langle M/n \rangle \) in a “molecule” (or the atoms in the formula unit of the crystal) and their average atomic weight. This model is useful to determine the temperature-dependent lattice thermal conductivity of materials. On the other hand, Clarke’s model is very advantageous for calculating the temperature-independent minimum thermal conductivity of compounds. Slack’s equation for calculating the lattice thermal conductivity is

\[
\kappa_{ph} = A \frac{M_{av} \theta_D^3 \delta}{\gamma^n \nu^{1/3} T}
\]  

(16)

In this formulation, \( M_{av} \) is the average atomic mass in kg mol\(^{-1}\), \( \theta_D \) is the Debye temperature in K, \( \delta \) is the cubic root of average atomic volume in \( m \), \( n \) is the number of atoms in a conventional unit cell, \( T \) is the temperature in K, and \( \gamma \) is the Grüneisen parameter, which is calculated from the Poisson’s ratio with the equation

\[
\gamma = \frac{3(1 + \nu)}{2(2 - 3\nu)}
\]  

(17)

The factor \( A(\gamma) \) due to Julian\(^{64} \) can be obtained as

\[
A(\gamma) = \frac{5.720 \times 10^7 \times 0.849}{2 \times (1 - 0.514/\gamma + 0.228/\gamma^2)}
\]  

(18)

The lattice thermal conductivity of V₂SnC calculated at room temperature (300 K) is listed in Table 6 and its temperature dependence is shown in Fig. 9. Table 5 also lists the literature values for other existing M₂SnC phases. Lattice thermal conductivity is highly sensitive to the Debye temperature. As the...
Debye temperature agrees fairly with the experimental value for the theoretical results with the GGA functional within the CASTEP and VASP codes, the room temperature lattice thermal conductivity calculated with the same functional within the same codes is expected to be consistent with the experiment if it is done in future. The reliability of Slack model has been established for MAX phases as their calculated lattice thermal conductivity agrees fairly well with the experimental values. For instance, the calculated (experimental) lattice thermal conductivity at 1300 K for Ta₄AlC₃ and Nb₂AlC₃ are 5 (6) W m⁻¹ K⁻¹ and 7 (7) W m⁻¹ K⁻¹, respectively. The lattice thermal conductivity at room temperature for M₂SnC MAX phases ranges from 14 to 30 W m⁻¹ K⁻¹ within the CASTEP-GGA calculations, which does not exceed the typical range for MAX phases. Fig. 9 exhibits the gradual decrease of lattice thermal conductivity of M₂SnC with the increase of temperature. The new phase V₂SnC has lattice thermal conductivities very close to those of Lu₂SnC for the whole range of temperatures. Lu₂SnC is already predicted as better TBC materials among M₂SnC (M = Lu, Ti, Nb, Zr, Hf) phases. Therefore, the new phase V₂SnC is expected to be a promising TBC material as Lu₂SnC.

The theoretical lower limit of intrinsic thermal conductivity of a material at high temperature is defined as its minimum thermal conductivity. The phonons become unpaired at high temperature and hence the heat energy is transferred to the adjacent atoms. In this situation, the mean free path of phonons is supposed to be the average interatomic distance. According to this approximation, different atoms can be substituted within a molecule with an equivalent atom having average atomic mass of M/n (n is the number of atoms in a primitive cell). A single “equivalent atom” within the cell never exhibits optical modes and hence it can be used to derive a formulation to determine the minimum thermal conductivity κₘᵢₙ at high temperature, as Clarke described in his model:

\[
\kappa_{\text{min}} = \frac{k_B n}{M} \frac{n N_A \rho}{M}
\]  
(19)

The symbols used in this expression carry the same meanings of those used in eqn (4). The minimum thermal conductivity calculated for the new MAX phase V₂SnC is listed in Table 6 along with literature values for other M₂SnC MAX phases. In the similar fashion of other properties, the minimum thermal conductivity calculated with GGA functional within CASTEP and VASP codes show more consistency than other results listed in Table 6. For comparison, we have another theoretical result of 0.755 W m⁻¹ K⁻¹ for Nb₂SnC,⁴⁴ which is identical to 0.76 W m⁻¹ K⁻¹ obtained in the present and a previous⁴⁶ calculations with GGA within CASTEP and VASP codes. The new phase has the highest value of 1.20 W m⁻¹ K⁻¹ among M₂SnC phases considering same functional within same code, which is very close to 1.13 W m⁻¹ K⁻¹ of a promising TBC material, Y₄Al₂O₉. Additionally, the ultralow minimum thermal conductivity of 1.25 W m⁻¹ K⁻¹ is used for selecting appropriate materials for TBC applications.⁴⁶ Therefore, M₂SnC phases including new phase V₂SnC have the possibility to be promising TBC materials.

3.5. Vibrational properties

To verify the dynamical stability of the newly synthesized V₂SnC MAX phase, the phonon dispersion and phonon density of states are investigated. The phonon dispersion curve is shown in the left panel of Fig. 10. There is no negative phonon frequency in the whole Brillouin zone. The absence of negative phonon frequency ensures the absence of soft phonon modes, indicating that the phase V₂SnC is dynamically stable against the mechanical perturbation at ambient state like the other existing M₂SnC phases.⁴² 211 MAX phases have eight atoms in their unit cell, which lead to 24 vibrational modes including three acoustic and 21 optical modes. The lower branches correspond to the acoustic modes (orange) and the upper branches with frequencies greater than 2 THz correspond to the optical modes (light blue). Lower optical branches overlap with the acoustic branches and consequently there is no phononic band gap between the acoustic and optical branches. The zero phonon frequency of the acoustic modes at the Γ point is another indication of dynamical stability of the V₂SnC MAX phase. The phonon DOS shown in the right panel of Fig. 10, reveals that the acoustic and lower optical modes arise due to the vibration of heavier atoms Sn and V. The higher optical
modes mainly originate from the vibration of lighter atom C. Acoustic phonon is caused by the coherent vibrations of atoms in a lattice outside their equilibrium position. On the other hand, when an atom moves to the left and its neighbour to the right, the optical phonon is originated due to the out-of-phase oscillation of the atom in a lattice. Optical phonons control the most of the optical properties of crystals.

3.6. Vickers’ hardness

Herein, the theoretical method based on Mulliken population developed by Gou et al.\textsuperscript{40} is used to calculate the Vickers’ hardness of partial metallic compounds. Within this method, the bond hardness $H_b^{\text{M}}$ is calculated as:

$$H_b^{\text{M}} = 740 \left( P^m - P^w \right) \left( \frac{v^w}{v^m} \right)^{-5/3} \tag{20}$$

where $P^m$ is the Mulliken overlap population of the $\mu$-type bond, $P^w$ is the metallic population and can be calculated with the unit cell volume $V$ and the number of free electrons in a cell, $n_{\text{free}}$ as follows: $n_{\text{free}} = \int_{V}^\infty N(E)dE$ and $P^w = \frac{n_{\text{free}}}{V}$. $E_p$ and $E_F$ are the energy at the pseudogap and at the Fermi level, respectively, $v^w$ is the volume of metallic bond and is calculated from the bond length $d^w$ of $\mu$-type and the number of bonds $N_v$ of $v$ type per unit volume using the equation $v^w = (d^w)^3/\sum (d^w)^3 N_v^w$. Then, the theoretical Vickers hardness for complex multilayer crystal can be determined as a geometric average of all bond hardness values as follows:

$$H_v = \left( \prod_n H_b^{\text{M}_n} \right)^{1/\sum_n n^m} \tag{21}$$

where $n^m$ represents the number of $\mu$-type bonds. The Vickers’ hardness calculated for $\text{M}_2\text{SnC}$ including new phase $\text{V}_2\text{SnC}$ is listed in Table 6. The new phase $\text{V}_2\text{SnC}$ has highest Vickers’ hardness in the $\text{M}_2\text{SnC}$ family. There are two sets of experimental values for $\text{T}_2\text{SnC}, \text{Zr}_2\text{SnC}, \text{Hf}_2\text{SnC}$, and $\text{Nb}_2\text{SnC}$\textsuperscript{35,70} The determined values show deviations from one set to another, except in the case of $\text{T}_2\text{SnC}$. Indeed, the determined values depend on the purity of the sample, instrumental set up and error. The present theoretical values (refer to Table 7) also differ from the experimental values. The temperature of the sample may be an additional reason. The theoretical $H_v$ of $\text{M}_2\text{SnC}$ ranges from 0.2 to 2.9 GPa. It is worth mentioning that the measured values of $H_v$ for MAX phases range from 2 to 8 GPa.

The theoretical $H_v$ of $\text{Lu}_2\text{SnC}$ is very small compared to the lower limit of measured value for MAX phases. The reason may be the absence of typical $M$–$C$ bond in the structure of $\text{Lu}_2\text{SnC}$. This also reduces the elastic constants, elastic moduli and melting and Debye temperature in $\text{Lu}_2\text{SnC}$. Consequently, $\text{Lu}_2\text{SnC}$ is the most soft and easily machinable compound in $\text{M}_2\text{SnC}$ as well as in MAX family. Indeed, the hardness of MAX phases is very small compared to their corresponding binary phases. Low hardness of MAX phases makes them machinable compounds. All phases in $\text{M}_2\text{SnC}$ family are easily machinable compared to many other MAX phases.

3.7. Defect processes

Frenkel defect energies provide the information regarding nuclear application of a material as the low pair formation energy is linked to a higher content of more persistent defects. These in turn cause the loss of ordering in the structure of a crystal. An accumulation of defects in a crystal that are formed by the displacement cascades are indicative of radiation tolerance of the material.\textsuperscript{71,72} In Table 8, the relations (1–3) are the key reactions for the Frenkel defects in Kröger–Vink notation\textsuperscript{73} for $\text{M}_2\text{SnC}$ phases.

Antisite defects are point defects formed due to either recombination or occupation of atoms at alternative lattice sites during radiation damage.\textsuperscript{74} Low energy antisite formation energy indicates that a major population of residual defects will persist in a material, as a net reduction of defect mobility arises due to change of an interstitial into an antisite.\textsuperscript{75,76} The antisite formation mechanisms are given by the reactions (4)–(6) in Table 8.

Displacive radiation causes an athermal concentration of Frenkel pairs, as it is assumed that the radiation tolerance of materials depends on the resistance to form persistent populations of Frenkel (and antisite) defects.\textsuperscript{77} In this context, high defect energy is indicative of radiation tolerance. In a previous study of $\text{M}_2\text{SnC}$ ($M = \text{Lu, Ti, Zr, Hf, and Nb}$) phases, $\text{Nb}_2\text{SnC}$ is predicted as most radiation tolerant MAX phase in these systems.\textsuperscript{3} If the new phase $\text{V}_2\text{SnC}$ is included in these systems $\text{Nb}_2\text{SnC}$ remains at the same position. Comparing with other $\text{M}_2\text{SnC}$ phases, the radiation tolerance in $\text{V}_2\text{SnC}$ is better than $\text{Lu}_2\text{SnC}$ and lower than remaining ones.

Although the $M$ interstitials, according to reaction (9), will recombine with $V_{\text{Sn}}^\text{0}$ to form $M$ antisites for all the $\text{M}_2\text{SnC}$ MAX phases studied here, there will be very little concentration of $M$.\textsuperscript{77}

### Table 7: Bond number $n^m$, bond length, $d^w$ (Å), bond population $P^m$, bond volume $v^w$ (Å$^3$), bond hardness $H_b^{\text{M}}$ (GPa), metallic population $P^w$, and hardness $H_v$ (GPa) of $\text{M}_2\text{SnC}$ MAX phases

| Compound | Bond | $n^m$ | $d^w$ (Å) | $P^m$ | $P^w$ | $v^w$ (Å$^3$) | $H_b^{\text{M}}$ (GPa) | $H_v$ (GPa) |
|----------|------|-------|----------|-------|-------|-------------|---------------------|-----------|
| $\text{V}_2\text{SnC}$ | V–C | 4 | 2.0526 | 1.02 | 0.05432 | 27.30 | 2.9 | 2.9 |
| $\text{Ti}_2\text{SnC}$ | Ti–C | 4 | 2.1414 | 1.08 | 0.01325 | 30.00 | 2.7 | 2.7 | 3.5,71 3.5,79 |
| $\text{Zr}_2\text{SnC}$ | Zr–C | 4 | 2.3118 | 1.05 | 0.01302 | 36.18 | 1.9 | 1.9 | 3.5,71 3.9,79 |
| $\text{Lu}_2\text{SnC}$ | Sn–C | 4 | 4.3478 | 0.12 | 0.00348 | 41.82 | 0.2 | 0.2 |
| $\text{Hf}_2\text{SnC}$ | Hf–C | 4 | 2.3158 | 1.39 | 0.00541 | 35.73 | 2.6 | 2.6 | 3.8,79 4.5,79 |
| $\text{Nb}_2\text{SnC}$ | Nb–C | 4 | 2.2014 | 0.99 | 0.00139 | 31.98 | 2.3 | 2.3 | 3.8,79 3.5,79 |
in the first place due to the very high reaction energies of reaction (1) listed in Table 8. Under equilibrium conditions, this will effectively render reaction (7) practically irrelevant. Similar arguments are also applicable for the other antisite reactions (8) and (9). These reactions may become pertinent in the case of a non-equilibrium environment (i.e., under irradiation) where an increased defect concentration is feasible. In this environment, it is expected that M₄ will recombine with V′ₘ to produce M₄ antisites. Moreover, the creation of Cₘn through the reaction (8) should be anticipated for Ti₄Sn₃. After irradiation, these processes may only be relevant, given that the formation energies of the M₄ defecta according to the Frenkel reaction (relation-(1)) are high for all the M₂Sn₃ MAX phases studied here (6.40–9.34 eV, refer to Table 8). The processes considered for the displacement of lattice atoms by interstitials (reactions (13)–(18)) are all positive in energy. The new phase requires lowest energy in Schottky reaction. From an experimental point of view, the radiation tolerance and oxidation resistance of M₂Sn₃ phases have to be determined at high temperature. A detailed understanding of the radiation tolerance of V₂Sn₃ requires systematic experimental work and simulation over a range of timescales and system sizes.

4. Conclusions

In summary, the density functional theory is employed to investigate the phase stability and physical properties of a newly synthesized 211 MAX phase, V₂Sn₃ for the first time. The calculated results are compared with those of other existing M₂Sn₃ (M = Ti, Zr, Hf, Nb, and Lu) phases. The newly synthesized compound V₂Sn₃ has passed the mechanical, dynamic and thermodynamic stability tests. The new phase V₂Sn₃ is the second most capable phase to resist the deformation in M₂Sn₃ systems following the order: Nb₂Sn₃ > V₂Sn₃ > Hf₂Sn₃ > Ti₂Sn₃ > Zr₂Sn₃ > Lu₂Sn₃. It also has the second highest value of B and θ₀ and an intermediate value of G and E in the M₂Sn₃ family. V₂Sn₃ is softer than Ti₂Sn₃ and stiffer than other existing M₂Sn₃ MAX phases. V₂Sn₃ has potential to be etched into 2D MXene like the other M₂Sn₃ phases. V₂Sn₃ and Nb₂Sn₃ are ductile and damage tolerant and the remaining phases are brittle in nature. The directional dependence of E, β, G and ν of M₂Sn₃ is calculated. All M₂Sn₃ phases show directional dependence of E, G, and ν in the xz and yz planes. Ti₂Sn₃ and Lu₂Sn₃ show almost directional independency on β. Elastic anisotropy in V₂Sn₃ is higher than Ti₂Sn₃ and less than the other M₂Sn₃ phases. The band structure and Fermi surface are indicative of possible superconductivity of V₂Sn₃. V₂Sn₃ is anticipated to be a promising TBC material as Lu₂Sn₃ among M₂Sn₃ phases. V₂Sn₃ is more radiation tolerant than Lu₂Sn₃ and less than the remaining other M₂Sn₃ phases.

Authors contribution

M. A. Hadi: conceptualization, data curation, investigation, methodology, formal analysis, writing – original draft. M. Dahlqvist: software, formal analysis, review & editing; S.-R. G. Christopoulos: investigation, data curation; S. H. Naqbi: project administration, review & editing; A. Chronos: formal analysis, writing, review & editing. A. K. M. A. Islam: formal analysis, review & editing.

Data availability

Supplementary data will be made available on request.
Conflicts of interest

There are no conflicts of interest to declare.

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