Phase stability of the nanolaminates $V_2Ga_2C$ and $(Mo_{1-x}V_x)_{2}Ga_{2}C$ from first-principles calculations†

A. Thore,* A. Dahlgqvist,* B. Alling† and J. Rosen

We here use first-principles calculations to investigate the phase stability of the hypothetical laminated material $V_2Ga_2C$ and the related alloy $(Mo_{1-x}V_x)_{2}Ga_{2}C$, the latter for a potential parent material for synthesis of $(Mo_{1-x}V_x)_{2}C$, a new two-dimensional material in the family of so called MXenes. We predict that $V_2Ga_2C$ is thermodynamically stable with respect to all identified competing phases in the ternary $V$–Ga–C phase diagram. We further calculate the stability of ordered and disordered configurations of Mo and V in $(Mo_{1-x}V_x)_{2}Ga_{2}C$ and predict that ordered $(Mo_{1-x}V_x)_{2}Ga_{2}C$ for $x \leq 0.25$ is stable, with an order–disorder transition temperature of $\sim 1000$ K. Furthermore, $(Mo_{1-x}V_x)_{2}Ga_{2}C$ for $x = 0.5$ and $x \geq 0.75$ is suggested to be stable, but only for disordered Mo–V configurations, and only at elevated temperatures. We have also investigated the electronic and elastic properties of $V_2Ga_2C$, the calculated bulk, shear, and Young’s modulus are 141, 94, and 230 GPa, respectively.

I. Introduction

In a recent paper by Hu et al., the discovery of a new crystalline phase, $Mo_2Ga_2C$, was reported, suggested to be the first member of a family of hitherto unknown materials closely related to the $M_{n+1}A_nX_n$ (MAX) phase family. The latter consists of a large number of hexagonal, layered materials based on a transition metal $[M]$, an A-group element $[A]$ and C or N $[X]$, which display a combination of metallic and ceramic properties. The structure of $Mo_5Ga_4C_3$ has been further investigated by Lai et al., who used a combination of theoretical calculations and experimental measurements to determine the structure, showing that the phase is indeed very similar to the MAX phase $Mo_2GaC$, with C atoms residing between the Mo layers in an octahedral position and the Ga atoms being stacked in a simple hexagonal arrangement.

$Mo_2GaC$ and $Mo_2Ga_2C$ have been synthesized in bulk as well as thin film form, however, only the latter material has been converted to $Mo_2C$, a so called MXene. Experimental results strongly suggest that $Mo_2GaC$, to date the only known Mo-containing ternary MAX phase, cannot be used for this purpose, even though MXenes, which comprise a class of two-dimensional materials, are typically obtained from MAX phases through selective etching of the A layer. The properties of $Mo_2C$ remains to be explored, although the first report on the topic suggests that it exhibits 2D superconductivity, based on the observation that the critical magnetic field is significantly increased when the field direction with respect to the plane of the film is changed from perpendicular to parallel.

To form a solid solution of two elements on a sublattice – in particular elements with different numbers of valence electrons – opens up for the possibility of tailoring the physical properties, something which has previously been demonstrated for quaternary MAX phases. For example, incorporation of 20 at% of V on the M sublattice of $Ti_2AlC$ leads to improvements in Vicker’s hardness, flexural strength, and shear strength. Motivated by this we here investigate and predict the phase stability as well as the electronic and elastic properties of a new $M_2A_2X$ phase (or 221 phase) with a single element on the M sublattice, $V_2Ga_2C$. We further investigate the stability of a 221 alloy $(Mo_{1-x}V_x)_{2}Ga_{2}C$ for different $Mo_{1-x}V_x$ concentrations.

Apart from the possibility of tuning of properties in $(Mo_{1-x}V_x)_{2}Ga_{2}C$ for different stoichiometries, synthesis of this phase would provide a promising experimental pathway for realizing 2D $(Mo_{1-x}V_x)_{2}C$, a hypothetical new MXene alloy. While it is possible to obtain $V_2C$ by etching away the Al layer in the MAX phase $V_2AlC$, the requirement of $Mo_2GaC$ for synthesis of $MoC$ suggests that the parent phase for $(Mo_{1-x}V_x)_{2}C$ is $(Mo_{1-x}V_x)_{2}Ga_{2}C$, and not the corresponding MAX phase alloy. The here presented results predict that the new phases $V_2Ga_2C$ as well as $(Mo_{1-x}V_x)_{2}Ga_{2}C$ are stable.

II. Calculation details

All calculations were carried out within the framework of density functional theory (DFT) as implemented in the Vienna ab initio
simulation package (VASP),\textsuperscript{11-14} using the Perdew–Burke–Ernzerhof generalized gradient approximation (PBE-GGA) as the exchange–correlation energy functional.\textsuperscript{15} The plane wave cutoff energy for the structural relaxations was set to 400 eV, and Monkhorst-Pack grids were used for the Brillouin zone samplings. The free energy convergence criterion for all pure phases was 0.1 meV per atom, whereas for the alloy it was chosen to be 0.5 meV per atom due to the requirement of large supercells (4 × 4 × 1, containing 160 atoms). The dynamical matrix of V\textsubscript{2}Ga\textsubscript{2}C was calculated using \Gamma-centered density functional perturbation theory (DFPT), and the phonon dispersion was extracted with the help of the PHONOPY software package.\textsuperscript{16,17}

All phase stability predictions in this work are based on a method for convex hull construction developed by Dahlgvist \textit{et al.} which combines first-principles calculations with a linear optimization procedure (the simplex algorithm).\textsuperscript{18} This method has previously been successfully used to predict the existence of several MAX phases,\textsuperscript{19-21} and it also reproduces the stability of several already synthesized MAX phases,\textsuperscript{19} as well as the stability of Mo\textsubscript{2}Ga\textsubscript{2}C.\textsuperscript{3,22}

For ordered \((\text{Mo}_{1-x}\text{V}_{x})_{2}\text{Ga}_{2}C\), the supercells were created using the special quasirandom structure (SQS) methodology developed by Zunger \textit{et al.}\textsuperscript{23} The same approach was used for competing phases that were alloyed on one or more sublattices, and/or contained vacancies. For ordered \((\text{Mo}_{1-x}\text{V}_{x})_{2}\text{Ga}_{2}C\), the enthalpies of a number of different, manually constructed M sublattice configurations were calculated and compared, all of which are listed in Table S2 in ESI.\textsuperscript{†}

The enthalpy of formation of V\textsubscript{2}Ga\textsubscript{2}C and ordered \((\text{Mo}_{1-x}\text{V}_{x})_{2}\text{Ga}_{2}C\), which was calculated through the linear optimization procedure described in ref. 22, can be expressed as

\[
\Delta H_{\text{cp}} = H_{221} - H_{\text{cp}},
\]

where \(H_{221}\) is the enthalpy of the 221 phase and \(H_{\text{cp}}\) is the total enthalpy of the set of most competing phases. Formally, \(H_{\text{cp}}\) is defined as

\[
\min H_{\text{cp}}(b^M, b^A, b^X) = \sum x_i H_i,
\]

where \(b^M, b^A, b^X\) is the amount of M, A, and X atoms in the set of competing phases is the same as in the 221 phase, which means that the \(x_i\)s are constrained in the following way:

\[
x_i \geq 0; \quad \sum x_i b_i^M = b^M, \quad \sum x_i b_i^A = b^A, \quad \sum x_i b_i^X = b^X.
\]

For the disordered 221 alloy and phases with vacancies, the enthalpy is replaced at finite temperature \(T\) by the Gibbs free energy,

\[
G = H - TS_c,
\]

where \(S_c\) is the configurational entropy, given by

\[
S_c = k_B \sum_j y_j \ln y_j.
\]

Here, \(y_j\) is the concentration of species \(i\). A necessary criterion for thermodynamic phase stability is that \(\Delta H_{\text{cp}} < 0\) (or \(\Delta G_{\text{cp}} < 0\)).

Lastly, the elastic properties of V\textsubscript{2}Ga\textsubscript{2}C were obtained using the method described by Fast \textit{et al.},\textsuperscript{24} where five elastic constants \(C_{11}, C_{12}, C_{13}, C_{33}, \) and \(C_{44}\) are obtained by first distorting the lattice in a stepwise fashion, then calculating the energy of each distortion step, given by

\[
E(V, \alpha) = E(V_0, 0) + V_0 \left( \sum_j \tau_j \alpha_j \zeta_{j} + \frac{1}{2} \sum_{j, l} C_{ij} \alpha_j \alpha_l \zeta_{jl} \right),
\]

where \(E(V_0, 0)\) is the energy of the unstrained lattice and \(\alpha_j\) are strain parameters, and finally carrying out a quadratic fit on the resulting energy-strain data. Each distortion step here corresponded to a strain of 1% in each direction, with a maximum strain of 2%, \textit{i.e.}, the strain parameters \(\alpha_j\) were allowed to assume the values 0, ±0.01, ±0.02.

\[\text{III. Results and discussion}\]

\[\text{A. Phase stability}\]

The topmost and bottom row of Table 1 contain the formation enthalpies, the lattice parameters, and the respective sets of most competing phases at 0 K for the hypothetical phase V\textsubscript{2}Ga\textsubscript{2}C and the recently synthesized nanolaminate Mo\textsubscript{2}Ga\textsubscript{2}C.\textsuperscript{3} The crystal structure of these phases is shown in Fig. 1. Out of a large number of considered competing phases (see Table S1 in ESI\textsuperscript{†}), the set of most competing phases with respect to V\textsubscript{2}Ga\textsubscript{2}C is found to consist of two experimentally verified phases, the MAX phase

<table>
<thead>
<tr>
<th>Phase</th>
<th>Set of most competing phases (0 K)</th>
<th>Lattice parameter (0 K)</th>
<th>(\Delta H_{\text{cp}}) (meV per atom)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{Mo}_2\text{Ga}_2\text{C})</td>
<td>(\text{Mo}_2\text{Ga}_2\text{C}), (\text{Mo}_2\text{Ga}_4)</td>
<td>Ordered: (a = 3.064)\textsuperscript{a} (a = 18.153)\textsuperscript{a}</td>
<td>-9\textsuperscript{a}</td>
</tr>
<tr>
<td>((\text{Mo}<em>{0.75}\text{V}</em>{0.25})_{2}\text{Ga}_2\text{C})</td>
<td>((\text{Mo}<em>{0.75}\text{V}</em>{0.25})_{2}\text{Ga}_2\text{C}), (\text{Mo}_2\text{Ga}_2\text{C}), (\text{Mo}_2\text{Ga}_4), (\text{Mo}_4\text{Ga}_4)</td>
<td>Ordered: (a = 3.028) (a = 18.256)</td>
<td>-3.7</td>
</tr>
<tr>
<td>((\text{Mo}<em>{0.5}\text{V}</em>{0.5})_{2}\text{Ga}_2\text{C})</td>
<td>((\text{Mo}<em>{0.5}\text{V}</em>{0.5})_{2}\text{Ga}_2\text{C}), (\text{Mo}_2\text{Ga}_2\text{C}), (\text{Mo}_2\text{Ga}_4)</td>
<td>Ordered: (a = 3.003) (a = 18.062)</td>
<td>18.3</td>
</tr>
<tr>
<td>((\text{Mo}<em>{0.375}\text{V}</em>{0.625})_{2}\text{Ga}_2\text{C})</td>
<td>((\text{Mo}<em>{0.375}\text{V}</em>{0.625})_{2}\text{Ga}_2\text{C}), (\text{Mo}_2\text{Ga}_2\text{C}), (\text{Mo}_2\text{Ga}_4), (\text{Mo}_4\text{Ga}_4)</td>
<td>Ordered: (a = 2.957) (a = 18.092)</td>
<td>13.3</td>
</tr>
<tr>
<td>((\text{Mo}<em>{0.25}\text{V}</em>{0.75})_{2}\text{Ga}_2\text{C})</td>
<td>((\text{Mo}<em>{0.25}\text{V}</em>{0.75})_{2}\text{Ga}_2\text{C}), (\text{V}_2\text{Ga}_2\text{C}), (\text{V}_2\text{Ga}_4)</td>
<td>Ordered: (a = 2.946) (a = 17.861)</td>
<td>-0.6</td>
</tr>
</tbody>
</table>

\textsuperscript{a}Ref. 3.
V$_2$GaC and the rhombohedral binary phase V$_2$Ga$_{41}$, and the hypothetical phase V$_8$Ga$_4$C$_2$. The latter belongs to the same space group as V$_2$Ga$_2$C ($P6_3/mmc$), but contains two V$_6$C octahedra between each Ga bilayer instead of one, similar to a MAX phase with a 312 stoichiometry.

Both V$_2$Ga$_2$C and Mo$_2$Ga$_2$C fulfill the criterion that $\Delta H_{cp} < 0$, although the formation enthalpy of $-0.6$ meV per atom for V$_2$Ga$_2$C is close to zero and could therefore hypothetically become positive if temperature dependent effects such as lattice vibrations are also included in the calculations. However, in a recent study we showed that, for the structurally closely related MAX phase Ti$_2$AlC, the temperature dependent effects cancel each other out. Further, as shown in Fig. 2, the phonon dispersion indicates that V$_2$Ga$_2$C is dynamically stable as there are no imaginary frequencies and thus no imaginary phonon modes present. The phase also fulfills the three criteria for mechanical stability, which for a hexagonal phase are the inequalities $C_{44} > 0$, $C_{11} > |C_{21}|$, and $(C_{11} + C_{12})C_{33} > 2C_{13}^2$. The values of the elastic constants can be found in Section IIIC, Table 3.

We have also investigated the phase stability of the quaternary alloy (Mo$_1$-$x$V$_x$)$_2$Ga$_2$C. Fig. 3 shows the isostructural Gibbs free energy of formation (as defined in eqn (1), with $G_{221}$ substituted for $H_{221}$) for chemically disordered (Mo$_1$-$x$V$_x$)$_2$Ga$_2$C with respect to the two end members Mo$_2$Ga$_2$C and V$_2$Ga$_2$C, for temperatures ranging from 0 to 1500 K. Also included in the figure are the formation enthalpies for chemically ordered (Mo$_1$-$x$V$_x$)$_2$Ga$_2$C, for a number of different V concentrations $x$ on the M sublattice. A common feature of all identified lowest-energy ordered configurations of (Mo$_1$-$x$V$_x$)$_2$Ga$_2$C is that the Mo and V atoms segregate into single element M layers. As shown in Fig. 4, the preferred M layer sequence for $x = 0.25$ and $x = 0.5$ is 6Mo2V and MoVMoV, respectively. The sequences for the other considered concentrations are 2Mo4V2Mo4V ($x = 0.33$), 4Mo2V4Mo2V ($x = 0.67$), 2Mo4V2Mo4V ($x = 0.33$), 4Mo2V4Mo2V ($x = 0.67$).
and 2Mo6V (x = 0.75). Ordered (Mo0.75V0.25)2Ga2C outcompetes both a linear combination of Mo2Ga2C and V2Ga2C and the disordered alloy for temperatures up to 1000 K. Above these temperatures, disordered (Mo0.75V0.25)2Ga2C is thermodynamically favored due to a significant configurational entropy contribution to the free energy.

The picture changes significantly when all known competing phases (~70, see Table S1 in ESI!) in the quaternary Mo–V–Ga–C phase diagram, together with hypothetical phases such as the binary phase MoGa4 (based on the existing, related cubic phase CrGa4), are included in the calculations. As seen in Table 1 for V concentrations x = 0.25, 0.5, and 0.75, the respective sets of most competing phases at 0 K are comprised of ternaries, binaries, and, for x = 0.25, pure carbon (graphite), which increases the formation enthalpies for both the ordered and disordered alloy. At 0 K only ordered (Mo0.75V0.25)2Ga2C is now stable, with ΔHcp = −3.7 meV per atom.

Fig. 5 combines all 0 K data in Table 1 with a superimposed line indicating Tdisorder (green open squares, right hand axis), i.e., the temperature at which the condition ΔGdisorder = ΔHcp is fulfilled and a disordered MoV solid solution on the M sublattice becomes energetically favorable (this notation was first introduced in ref. 27). Also indicated in the figure is TΔGcp=0 (solid line, teal open triangles), where ΔGcp=0 is the temperature at which the disordered alloy first becomes stable with respect to its set of most competing phases. For x = 0.5 and 0.75, only disordered (Mo0.75V0.25)2Ga2C is indicated as potentially stable at elevated temperatures, with TΔGcp=0 ≈ 2100 and 1750 K, respectively. For x = 0.25, on the other hand, both ordered and disordered (Mo0.75V0.25)2Ga2C is stable, with TΔGcp=0 ≈ 880 K, and TΔGcp=0 ≈ 1000 K. Since common bulk synthesis temperatures are 1200–1600 °C (1473–1873 K), these results thus suggest that synthesis of the disordered quaternary alloy (Mo0.75V0.25)2Ga2C should at least be possible for x ≤ 0.25 and x ≥ 0.75. For the former concentration range, it might be possible to synthesize an ordered configuration at temperatures below 880 K.

It should be noted that for all three V concentrations, MoGa4 (a phase not to be confused with Mo6Ga31, which has almost the same stoichiometry, but a different structure) is one of the most competing phases not only at 0 K, but also at and above TΔGcp=0. This is a binary phase which has, to the best of our knowledge, not yet been experimentally verified. This might be because of a lack of trying, or because it does not form readily. If the latter is the case, the experimental window for synthesizing disordered (Mo0.75V0.25)2Ga2C (which would then be a metastable phase) expands significantly, with possible synthesis temperatures for x = 0.25, 0.5, and 0.75 starting at around 900, 1000, and 1500 K, respectively. These temperatures are indicated by the teal dashed line in Fig. 5.

Table 1 shows that the a and c lattice parameters decrease more or less linearly with a decreasing amount of Mo. The a parameter obeys Vegard’s law quite closely, while this is not apparent for the c parameter. Finally, the differences between corresponding parameters for the ordered and the disordered alloy are quite small.

B. Electronic properties of V2Ga2C

Fig. 6 shows the electronic band structure and the total and atomic densities of states (tDOS and aDOS, respectively) for V2Ga2C and V2GaC. The band structure of V2Ga2C exhibits considerable anisotropy around the Fermi level, with several band crossings in the A–L, M–Γ, Γ–K, and H–A reciprocal space directions, but none in the Γ–A, L–M, and K–H directions. Band structure anisotropy, which together with electron–phonon coupling anisotropy28 is often an indicator of anisotropic conductive properties, is a common feature of MAX phases, including V2GaC and the 221 phase Mo3Ga2C3,29,30.

Qualitatively, the tDOS and aDOS for V2Ga2C are very similar compared to V2GaC. The states around E Fermi in both phases are mostly dominated by V electrons (more specifically V 3d electrons). Evidence of V–C and weak V–Ga bonding is seen at around −3.5 eV, where there is overlap between the V, Ga, and C peaks; slightly stronger V–Ga bonds should be expected in the intervals from −2 eV to −1 eV, where more Ga states are present in both V2Ga2C and V2GaC.

A Bader charge analysis has been carried out in order to investigate the charge transfer in V2GaC, which is a consequence of the differences in electronegativity between the constituting elements (1.6 for V and Ga; 2.5 for C).31 As seen in Table 2, a charge of 0.5 e is transferred from the [V2C] blocks to the Ga layers, whereas within the [V2C] blocks, 1.73 e is transferred from V2 to C.

Also listed in Table 2 are the partial charges of the M, A, and X atoms in V2GaC, Mo2Ga2C, and Mo2GaC. The [M2C] → Ga charge transfer is smaller in the 221 phases than in the corresponding MAX phases, as the former contain two Ga atoms per [M2C] block instead of one. However, this fact alone cannot account for the observed difference, since the transferred
charge per Ga atom in the 221 phases is less than half the amount of charge transferred in the MAX phases. For V$_2$Ga$_2$C, the discrepancy is 0.05 e (0.5 e vs. 0.55 e), while it is 0.09 e for Mo$_2$Ga$_2$C (0.08 e vs. 0.17 e). These discrepancies are likely caused by differences in the electronic structure, and they may suggest that the ionic components of the bonds between the [M$_2$C] blocks and the Ga layers are slightly weaker in the 221 phases than in the corresponding MAX phases.

C. Elastic properties of V$_2$Ga$_2$C

The Voigt bulk ($B_V$) and Voigt shear modulus ($G_V$) can be calculated from the five elastic constants $C_{11}$, $C_{12}$, $C_{13}$, $C_{14}$, and $C_{33}$ discussed in Section II. The moduli are related to these constants as:

$$B_V = \frac{2}{9} (C_{11} + C_{12} + 2C_{13} + C_{33}/2)$$  \hspace{1cm} (6)

and

$$G_V = 115(2C_{11} + C_{33} - C_{12} - 2C_{13}) + 15(2C_{44} + 12C_{11} - C_{12})$$  \hspace{1cm} (7)

From $B_V$ and $G_V$, Young's modulus ($E$) and Poisson's ratio ($\nu$) can be calculated:

$$E = \frac{9B_V G_V}{3B_V + G_V}$$  \hspace{1cm} (8)

$$\nu = \frac{3B_V - 2G_V}{2(3B_V + G_V)}$$  \hspace{1cm} (9)

The three moduli given by eqn (6)–(8) are shown for V$_2$Ga$_2$C in the three left panels of Fig. 7, together with the corresponding theoretical data for V$_2$Ga$_2$C, Mo$_2$Ga$_2$C, and Mo$_2$GaC, for comparison. In order to bound the moduli, we have used four different exchange–correlation functionals: PBE, LDA, and the two revised PBE functionals PBEsol and RPBE.\textsuperscript{32,33} The same functionals have been used to calculate the lattice parameters for all phases, as seen in the four right panels of Fig. 7. The RPBE functional yields the largest lattice parameters and thus sets a lower bound for the moduli, while the LDA sets an upper bound as it yields the smallest parameters. As is also seen in the figure, the experimentally determined lattice parameters for V$_2$Ga$_2$C, Mo$_2$Ga$_2$C, and Mo$_2$GaC closely match those from the PBE and PBEsol calculations. This suggests that, if V$_2$Ga$_2$C is synthesized, the lattice parameters will likely agree well with both the PBE and PBEsol calculations. We thus expect that these two functionals give the most accurate estimates of the elastic moduli out of the four functionals tested here.

In Table 3 we list the five elastic constants, the three moduli, and the Poisson’s ratios (eqn [9]) for V$_2$Ga$_2$C, V$_2$GaC, Mo$_2$Ga$_2$C, and Mo$_2$GaC, all obtained from calculations using the PBE exchange–correlation functional. As is seen in the table, V$_2$Ga$_2$C has similar moduli compared to Mo$_2$Ga$_2$C, but they are significantly lower (20–30%) than for V$_2$GaC. A decrease in the moduli is also observed for Mo$_2$Ga$_2$C compared to Mo$_2$GaC, as first reported in ref. 3.

At 0.23, Poisson’s ratio for V$_2$Ga$_2$C is 10% greater than for V$_2$GaC, and about 12% smaller than for Mo$_2$GaC.

The differences in the elastic properties of the 221 phases compared to the MAX phases can be attributed to the additional Ga layers in the former. Part of the explanation might be a weaker ionic component of the bonds between the [M$_2$C] blocks and Ga layers compared to the MAX phases, which was discussed in Section IIIB. Likely to be more significant, however, are the Ga–Ga bonds along the c axis in the 221 phases, which should be mainly metallic in character and presumably rather weak compared to the vertical V–Ga, V–C, and V–V bonds.
IV. Conclusions

We have calculated the phase stability of V$_2$Ga$_2$C and of the related alloy (Mo$_{1-x}$V$_x$)$_2$Ga$_2$C for three different V concentrations: $x = 0.25$, 0.5, and 0.75. The formation enthalpy of V$_2$Ga$_2$C with respect to its set of most competing phases is $-0.6$ meV per atom, which suggests that it is thermodynamically stable. Furthermore, V$_2$Ga$_2$C was found to be dynamically as well as mechanically stable.

For (Mo$_{1-x}$V$_x$)$_2$Ga$_2$C and $x \leq 0.25$, phase stability is indicated both for an ordered and a disordered configuration on the M sublattice, where the latter is stabilized at around 1000 K. Phase stability is further indicated for disordered (Mo$_{1-x}$V$_x$)$_2$Ga$_2$C for $x = 0.5$ and $x \geq 0.75$, at temperatures of about 2100 and 1750 K, respectively.

We have also investigated the electronic and elastic properties of V$_2$Ga$_2$C. The layered nature of the crystal structure is reflected in the electronic band structure in the form of a distinct anisotropy, which is a possible indicator of anisotropic conductivity. The calculated Voigt bulk modulus is 141 GPa, the Voigt shear modulus 94 GPa, and Young’s modulus 230 GPa, which are lower values than for the corresponding MAX phase V$_2$GaC. A Bader analysis shows significant charge transfer within the [V$_2$C] blocks and a smaller transfer between the [V$_2$C] blocks and the Ga layers in both V$_2$Ga$_2$C and the MAX phase counterpart V$_2$GaC. The differences in the elastic moduli between V$_2$Ga$_2$C and V$_2$GaC might be partly explained by a smaller [V$_2$C] → Ga transfer in V$_2$Ga$_2$C, but we speculate that the most important factor is weak interlayer bonding between the Ga layers in this phase.

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