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First-principles calculations of the electronic, vibrational, and elastic properties of the magnetic laminate Mn_2GaC

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In this paper, we report the by first-principles predicted properties of the recently discovered magnetic *MAX* phase Mn_2GaC . The electronic band structure and vibrational dispersion relation, as well as the electronic and vibrational density of states, have been calculated. The band structure close to the Fermi level indicates anisotropy with respect to electrical conductivity, while the distribution of the electronic and vibrational states for both Mn and Ga depend on the chosen relative orientation of the Mn spins across the Ga sheets in the Mn–Ga–Mn trilayers. In addition, the elastic properties have been calculated, and from the five elastic constants, the Voigt bulk modulus is determined to be 157 GPa, the Voigt shear modulus 93 GPa, and the Young's modulus 233 GPa. Furthermore, Mn_2GaC is found relatively elastically isotropic, with a compression anisotropy factor of 0.97, and shear anisotropy factors of 0.9 and 1, respectively. The Poisson's ratio is 0.25. Evaluated elastic properties are compared to theoretical and experimental results for $M_2\text{AC}$ phases where $M = \text{Ti, V, Cr, Zr, Nb, Ta}$, and $A = \text{Al, S, Ge, In, Sn}$. © 2014 AIP Publishing LLC.

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I. INTRODUCTION

MAX phases comprise a class of nanolaminated ternary materials with the general formula $M_{n+1}AX_n$ ($n = 1, 2, 3$), where M is a transition metal, A is an A -group element, and X is usually carbon or nitrogen. *MAX* phases were first discovered in the 1960s, when Nowotny and co-workers synthesized and characterized a large set of *MAX* phases with $n = 1$ (then denoted as "*H*-phases"),^{1,2} and, to date, more than 70 different *MAX* phases are known to exist. What characterizes this class of materials is a unique combination of metallic and ceramic properties that stems from the more metallic M – A and more covalent M – X bonds. With properties such as high electric conductivity, high ductility, creep resistance, and heat as well oxidation resistance, suggested potential applications range from electrical contacts and tool coatings, to more efficient combustion engines.^{3–5} With the recent discovery of the first magnetic *MAX* phases, this range can now be further widened to also include, e.g., spintronic applications.

Theoretical predictions of the existence of magnetic *MAX* phases have been around for a few years,^{6,7} but it was only recently that the first experimental evidence was reported. In 2013, three different magnetic *MAX* phases obtained through alloying between Cr and Mn on the M site were presented: $(\text{Cr}_{1-x}\text{Mn}_x)_2\text{GeC}$ ($x \sim 0.25$) by Ingason *et al.*,⁸ $\text{Cr}_{1-x}\text{Mn}_x\text{GaC}$ (where $0 < x < 0.5$) by Lin *et al.*,⁹ and $(\text{Cr}_{1-x}\text{Mn}_x)_2\text{AlC}$ ($x \sim 0.16$) by Mockute *et al.*^{10,11} These findings were followed by even more recent reports on these alloys.^{12–14} Later, Ingason *et al.* proceeded to synthesize Mn_2GaC ,¹⁵ the first

MAX phase with a hitherto unexplored M site element, Mn, since Nowotny's pioneering work. In the case of $(\text{Cr}_{1-x}\text{Mn}_x)_2\text{AlC}$,^{10,11} $(\text{Cr}_{1-x}\text{Mn}_x)_2\text{GeC}$,⁸ and Mn_2GaC ,¹⁵ the successful thin film synthesis was prompted by predictions of thermodynamic phase stability based on a first-principles approach developed by Dahlqvist *et al.*^{16,17}

In this work, we investigate selected physical properties of Mn_2GaC , which, due to its recent discovery, is still largely unexplored. The electronic, vibrational, and elastic properties are calculated from first principles, including an evaluation of the effect of different magnetic spin configurations of Mn_2GaC . Furthermore, the elastic properties are compared to those for $M_2\text{AC}$ phases where $M = \text{Ti, V, Cr, Zr, Nb}$, and Ta , and $A = \text{Al, S, Ge, In, and Sn}$.

II. CALCULATION DETAILS

The electronic band structure and electronic density of states was calculated within the framework of density functional theory (DFT),¹⁸ as implemented in the Vienna *ab initio* simulation package (VASP).^{19–22} The projector augmented wave method (PAW) was used to solve the Kohn–Sham equations,^{23,24} and the spin polarized Perdew–Burke–Ernzerhof generalized gradient approximation (PBE–GGA) was chosen as the exchange–correlation energy functional.²⁵

Structural relaxations were carried out using a plane wave cutoff energy of 400 eV and Γ centered Monkhorst–Pack grids for the Brillouin zone sampling, with a convergence criterion of 0.1 meV/atom with respect to the plane wave cutoff energy and number of k -points.

The phonon band structure and phonon density of states was obtained with the PHONOPY software package from force constant matrices calculated using the VASP implementation of density functional perturbation theory

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(DFPT).^{26,27} Sufficient convergence with respect to the forces was reached for a $3 \times 3 \times 1$ Mn_2GaC supercell.

To obtain the elastic properties, we used the method described by Fast *et al.*²⁸ Five different strains were applied to the hexagonal unit cell in order to attain the five independent elastic constants C_{11} , C_{12} , C_{13} , C_{33} , and C_{44} , given by the equation

$$E(V, \alpha) = E(V_0, 0) + V_0 \left(\sum_i \tau_i \alpha_i \xi_i + \frac{1}{2} \sum_{ij} C_{ij} \alpha_i \xi_i \alpha_j \xi_j \right), \quad (1)$$

where $E(V, \alpha)$ is the energy of the strained structure, $E(V_0, 0)$ is the energy of the unstrained structure, and the magnitudes of the strain parameters α_{ij} were chosen to be 0, ± 0.01 , and ± 0.02 , corresponding to 0, ± 1 , and $\pm 2\%$ strain, respectively. A quadratic fit was performed on the resulting energy–strain data to extract the elastic constants C_{ij} .

Based on the suggested low-energy magnetic spin configurations of Mn_2GaC in Refs. 15 and 29, we have included results for nonmagnetic (NM), ferromagnetic (FM), and two antiferromagnetic (AFM) spin configurations. In line with the notation in Ref. 30, the antiferromagnetic configurations (illustrated in Fig. 1) are designated as $\text{AFM} [0001]_4^A$ and $\text{AFM} [0001]_2^A$, corresponding to 4 and 2 consecutive M (here Mn) layers, respectively, with the same spin orientation before changing sign upon crossing an A (here Ga) layer. Note that the unit cell of the $\text{AFM} [0001]_4^A$ configuration is of size $1 \times 1 \times 2$ relative to the unit cells of the NM, FM, and $\text{AFM} [0001]_2^A$ configurations.

FIG. 1. Schematic representation of FM, $\text{AFM} [0001]_4^A$, and $\text{AFM} [0001]_2^A$ Mn_2GaC . For $\text{AFM} [0001]_4^A$, Ga 1,2 and Mn 1,2 represent inequivalent sites. Arrows indicate the relative spin orientation of the Mn atoms.

III. RESULTS AND DISCUSSION

A. Stability

The criterion for thermodynamic phase stability is that the energy of the investigated phase is lower than the energy of any stoichiometric linear combination of other competing phases within the same materials system. Since the number of competing phases can be quite large, it is not feasible to manually search for and test these combinations. A linear optimization method that automates this process has been developed by Dahlqvist *et al.*,^{16,17} and used to successfully confirm the existence of previously known MAX phases, as well as to predict the existence of new MAX phases.^{8,10,11,15,17,31} For example, as Fig. 2 shows, results from using this method accurately reflect what is experimentally known for $\text{Ti}_{n+1}\text{GaC}_n$ (synthesized: $n=1,2,3$), $\text{V}_{n+1}\text{GaC}_n$ (synthesized: $n=1$), and $\text{Cr}_{n+1}\text{GaC}_n$ (synthesized: $n=1$), and the results also correctly predict the existence of magnetic Mn_2GaC ($n=1$). It should be noted that while these results are all based on 0 K calculations, recent findings suggest that they would likely not be significantly altered by the addition of temperature dependent effects such as vibrational free energy, due to a mutual cancellation of these effects when the total free energy of the set of most competing phases is subtracted from that of the MAX phase.³²

The inset in Fig. 2 shows that the M atoms in both the Cr- and Mn-based MAX phases have strong local magnetic moments. These are obtained from the identified lowest energy spin configuration of each phase, which correspond to $\text{AFM} [0001]_4^A$ for Mn_2GaC ,²⁹ in-AFM1 for Cr_2GaC ,³⁰ and FM states for the hypothetical higher order Mn and Cr based MAX phases ($n=2,3$). The suggested collinear ground state magnetic configuration of Mn_2GaC is, however, as seen in Table I, nearly degenerate in energy with both the $\text{AFM} [0001]_2^A$ and the FM configuration. With respect to the identified set of most competing phases, which is comprised by FM Mn_3GaC , FM MnGa_4 , and C, the $\text{AFM} [0001]_4^A$ configuration has a formation enthalpy of -31 meV/atom, whereas $\text{AFM} [0001]_2^A$ and FM Mn_2GaC have formation enthalpies of -30 and -29 meV/atom, respectively.

FIG. 2. Stability trends for magnetic and nonmagnetic $\text{Mn}_{n+1}\text{GaC}_n$ phases ($M=\text{Ti}, \text{V}, \text{Cr}, \text{Mn}$): $\Delta H_{cp} < 0$ indicates phase stability. Inset: the local magnetic moments of the M atoms for the identified lowest energy spin configuration of each phase.

TABLE I. Magnetic configuration, most competing phases, formation enthalpy, and theoretical lattice parameters for Mn₂GaC.

Mn ₂ GaC	Magnetic configuration	Most competing phases	ΔH_{cp} (meV/atom)	Lattice parameters (Å)	
				a	c
Theory (0 K)	NM	Mn ₃ GaC, MnGa ₄ , C	+69	2.89	12.21
	FM	Mn ₃ GaC, MnGa ₄ , C	−29	2.90	12.29
	AFM [0001] ₂ ^A	Mn ₃ GaC, MnGa ₄ , C	−30	2.90	12.48
	AFM [0001] ₄ ^A	Mn ₃ GaC, MnGa ₄ , C	−31	2.90	12.41
Experiment (300 K) ^a	...	...	...	2.90	12.55

^aReference 15.

Mn₂GaC has a hexagonal lattice. However, while a *MAX* phase is usually described by space group *P6₃/mmc* (#194), this symmetry is broken by the magnetic order of AFM [0001]₄^A upon structural relaxation. Instead, the lattice assumes the symmetry of space group *Amm2* (#38). This is reflected in the geometry as the Mn 1 – Ga 1 – Mn 1 separation is slightly larger ($\sim 1.6\%$) than the corresponding Mn 2 – Ga 2 – Mn 2 distance.

Corroborating the conclusions from the thermodynamic phase stability calculations are the obtained positive frequencies for the phonon dispersion for AFM [0001]₄^A Mn₂GaC, discussed in Sec. III C. Furthermore, the criteria for mechanical stability, according to which the strain energy given by Eq. (1) has to be positive, are fulfilled.³³ For a hexagonal phase, these criteria can be expressed in terms of the elastic constants as

$$C_{44} > 0, \quad (2a)$$

$$C_{11} > |C_{12}|, \quad (2b)$$

and

$$(C_{11} + C_{12})C_{33} > 2C_{13}^2. \quad (2c)$$

The elastic constants are found in Table II, Sec. III D.

TABLE II. Calculated elastic constants (GPa) for four different *M*₂GaC phases (*M* = Ti, V, Ga, C) with different magnetic configurations. Data from this work appear in bold; the first row for each phase contains data for the suggested magnetic ground state.

Phase	Magnetic configuration	<i>C</i> ₁₁	<i>C</i> ₁₂	<i>C</i> ₁₃	<i>C</i> ₃₃	<i>C</i> ₄₄
Ti ₂ GaC	NM	305	73	66	261	102
	NM	303 ^a	66 ^a	63 ^a	263 ^a	101 ^a
V ₂ GaC	NM	331	70	116	298	139
	NM	334 ^a	81 ^a	111 ^a	299 ^a	138 ^a
Cr ₂ GaC	in – AFM1 ^b	313	72	107	321	119
	NM	323	81	125	336	130
	N/A	312 ^a	81 ^a	139 ^a	325 ^a	128 ^a
Mn ₂ GaC	AFM [0001] ₄ ^A	278	88	102	270	96
	AFM [0001] ₂ ^A	261	65	116	258	90
	FM	277	92	101	251	104
	NM	215	176	130	313	63

^aReference 39.^bReference 30.

B. Electronic properties

The electronic band structure and total density of states (TDOS) for AFM [0001]₄^A and FM Mn₂GaC is presented in Figs. 3(a) and 3(b). Immediately noticeable for AFM [0001]₄^A Mn₂GaC is that along the Γ – L, Γ – K, and H – A reciprocal space directions, there are several bands that cross the Fermi level, whereas no crossings occur along the Γ – A, L – M, and K – H directions. Band structure anisotropy around the Fermi level—which is here also seen for FM Mn₂GaC, albeit to a lesser extent—is commonly observed in *MAX* phases, and is suggested as an indication of anisotropic transport properties.³⁴ For this particular material, this would mean that one should expect charge carrier mobility to be significantly higher in-plane than in out-of-plane. We note that recent experimental results suggest that conductivity in *MAX* phases may be dependent on electron – phonon coupling, and that it is therefore this phenomenon rather than the electronic structure that dictates to which degree the phase is

FIG. 3. The electronic band structure and total density of states for Mn₂GaC. (a) AFM [0001]₄^A spin configuration. (b) FM spin configuration. Spin up and spin down states are given by red and grey lines, respectively. For AFM [0001]₄^A Mn₂GaC, the spin states overlap.

FIG. 4. Partial density of states for AFM $[0001]_4^A$ Mn_2GaC .

anisotropic with respect to electrical conductivity.^{35–37} As discussed in both Refs. 35 and 36, contrary to predictions from the calculated band structures, the investigated MAX phases show surprisingly weak conductive anisotropy. However, as structural optimization of the MAX phases needs to be undertaken for experimental evaluation of anisotropy, as well as further development of experimental procedures for evaluating the transport properties, this remains to be further explored.

The partial density of states (PDOS) for AFM $[0001]_4^A$ Mn_2GaC is shown in Figs. 4(a)–4(e), where Mn 1,2 and Ga 1,2 are defined as in Fig. 1, all C sites are equivalent. From -7 up to about -3.5 eV, there is a mix of Mn d , Ga s , and C p states. The Mn d and C p peaks that coincide at around -4.5 and -3.5 eV, and which correspond to the two flat bands seen in Fig. 3(a), are evidence of Mn d –C p bonding. The region above -3.5 eV is dominated by Mn d and Ga p states, mixed with a few Ga s states. The Mn d states are particularly abundant between -2 and 2 eV, while the Ga p states are mainly found between -3.5 and -1.5 eV.

The narrow Ga s peak seen in Fig. 4(e) at -1 eV is present only for Ga 2, i.e., when the surrounding Mn sheets have mutually parallel spins. Since there is also a sharp Mn d peak at -1 eV, this implies that for the Mn 2–Ga 2–Mn 2 tri-layers, one should be able to find relatively strong but highly localized Mn d –Ga s bonds at this energy. Further differences that result from the different magnetic environments around the Ga sheets (antiferromagnetic for Ga 1; ferromagnetic for Ga 2) are that the Ga 2 atoms have nonzero local magnetic moments, as reflected by the spin–splitting in Fig. 4(e), and that, for the Ga 1 atoms, there is an increase in the number of p states from -3 to 0 eV. Also, for both Mn 2 and Ga 2, the Fermi level is at a local maximum, something which is not seen either for Mn 1 or Ga 1. However, overall the TDOS around the Fermi level is populated mostly by Mn d states, and so conduction is likely to primarily involve Mn d electrons.

C. Vibrational properties

The phonon dispersion and phonon TDOS for AFM $[0001]_4^A$ Mn_2GaC is displayed in Fig. 5. With 16 atoms in the unit cell, there are 48 bands in total: 3 acoustic and 45 optical

FIG. 5. Phonon band structure and total density of states for AFM $[0001]_4^A$ Mn_2GaC .

bands. The peak frequency of the highest acoustic band is ~ 6 THz, while the frequency of the highest optical band oscillates around 20 THz.

The dispersion diagram can be separated into two main regions: One broad ranging from 0 to roughly 10 THz and one narrower from ~ 16 to ~ 20 THz. This separation is caused by the different mass of the three atomic species. As is seen in Figs. 6(a)–6(c), which show the partial phonon density of states (PDOS), the low frequency region is mainly occupied by the Mn and Ga atoms. The heavier Ga atoms dominate the lower half of this region, while the lighter Mn atoms dominate the upper half (the narrow Mn peak at ~ 9 THz corresponds to the flat bands seen at the same frequency in Fig. 5). The high frequency region is almost exclusively occupied by the lightest atomic species, C, with a PDOS showing two large peaks separated by a small frequency gap. Only a few states in this region are occupied by Mn atoms, while there are no discernible Ga states.

FIG. 6. PDOS for Mn and Ga in the Mn 1–Ga 1–Mn 1 and Mn 2–Ga 2–Mn 2 tri-layers. (a) Atomic vibrations in the x – y plane. (b) Vibrations along the z axis.

Figures 6(a) and 6(b) show that just as for the electronic DOS, there is a redistribution of the vibrational states across the Ga sheets where Mn spins change sign (Ga 1), although it is not as pronounced here. This redistribution may be explained by the varying Mn – Ga – Mn separation mentioned in Sec. III A, as this should affect the magnitude of the force constants. Further, by comparing Figs. 6(a) and 6(b), it is seen that the lower frequency Mn and Ga peaks are dominated by in-plane (xy) vibrations, while the right peaks consist of an even mix of in-plane (xy) and out-of-plane (z) vibrations. As can be seen for the C atoms in Fig. 6(c), there is an obvious split of out-of-plane (left peak) and in-plane (right peak) vibrations.

Although no experimental data for Mn₂GaC are available for comparison, the overall phonon PDOS is similar to theoretical data for other MAX phases, e.g., those reported for Ti₃SiC₂, Ti₃GeC₂, Ti₂AlN, Cr₂GeC, and Ti₄AlN₃ by Lane *et al.*³⁸

D. Elastic properties

While no experimental or theoretical data on the elastic properties of Mn₂GaC exist, theoretical data can be found for, e.g., Ti₂GaC, V₂GaC, Nb₂GaC, Ta₂GaC, and Cr₂GaC.^{39–41} In Table II, we list the five elastic constants for Mn₂GaC given by Eq. (1), including the corresponding data for Ti₂GaC, V₂GaC, and Cr₂GaC. The first row for each phase contains data for the suggested ground state magnetic configuration. To show the effect of magnetism for Cr₂GaC and Mn₂GaC, we have also included the elastic constants for the NM state.

As can be seen for both Cr₂GaC and Mn₂GaC, going from a nonmagnetic to a magnetic state can have a significant impact on the magnitude of the elastic constants. For example, the magnitude of C_{12} for AFM [0001]₄^A Mn₂GaC is only 50% of that for NM; for C_{44} , the corresponding difference is 33%. These differences then propagate to the three elastic moduli listed in Table III, as well as to the parameters A_c , A_{s1} , A_{s2} , ν , μ_D , and μ_M , which are defined in the discussion below.

Compared to the suggested ground state configurations of the other M_2 GaC phases, Mn₂GaC with AFM [0001]₄^A spin configuration (just Mn₂GaC from now on) has the lowest value of the elastic constants C_{11} and C_{44} , and the second lowest value of C_{13} and C_{33} , while it has the highest value of C_{12} . This has the effect that the Voigt bulk modulus,

$$B_V = \frac{2}{9}(C_{11} + C_{12} + 2C_{13} + C_{33}/2), \quad (3)$$

and the Voigt shear modulus,

$$G_V = 115(2C_{11} + C_{33} - C_{12} - 2C_{13}) + 15(2C_{44} + 12(C_{11} - C_{12})), \quad (4)$$

become low as well: B_V is the second lowest, and G_V is the lowest. This, in turn, yields the lowest Young's modulus, since it can be described by the equation,

$$E = \frac{9B_V G_V}{3B_V + G_V}, \quad (5)$$

which decreases with a simultaneous decrease of B_V and G_V .

In Table IV, we compare our calculated moduli for Mn₂GaC to the upper and lower values of the experimentally measured moduli for the M_2 AC phases listed in Ref. 42, and we see that the Voigt bulk and shear modulus for Mn₂GaC are fairly low, whereas the Young's modulus is intermediate in magnitude.

A way to quantify the elastic anisotropy of a material⁴⁹ is by calculating the compression anisotropy factor

$$A_c = \frac{C_{33}}{C_{11}}, \quad (6)$$

and the two shear anisotropy factors

$$A_{s1} = \frac{C_{11} + C_{33} - 2C_{13}}{4C_{44}} \quad (7)$$

and

TABLE III. Calculated Voigt bulk moduli B_V (GPa), Voigt shear moduli G_V (GPa), Young's moduli E (GPa), anisotropy factors A_c , A_{s1} , and A_{s2} , Poisson's ratio ν , ductility index μ_D , and machinability index μ_M for four M_2 GaC phases (M = Ti, V, Cr, and Mn). Data from this work appear in bold; the first row for each phase contains data for the suggested magnetic ground state.

Phase	Magnetic configuration	B_V	G_V	E	A_c	A_{s1}	A_{s2}	ν	μ_D	μ_M
Ti ₂ GaC	NM	142	108	259	0.86	1.06	0.88	0.20	1.31	1.40
	NM	139 ^a	109 ^a	260 ^a	0.87 ^b	1.09 ^b	0.85 ^b	0.19 ^b	1.28 ^a	1.38 ^a
V ₂ GaC	NM	174	126	304	0.90	0.71	1.07	0.21	1.38	1.25
	NM	175 ^a	125 ^a	302 ^a	0.90 ^b	0.74 ^b	1.09 ^b	0.21 ^b	1.40 ^a	1.27 ^a
Cr ₂ GaC	in – AFM1 ^c	169	116	283	1.03	0.88	0.99	0.22	1.46	1.41
	NM	183	120	296	1.04	0.79	1.07	0.23	1.53	1.41
	N/A	185 ^a	114 ^a	283 ^a	1.04 ^b	0.70 ^b	1.11 ^b	0.24 ^b	1.62 ^a	1.45 ^a
Mn ₂ GaC	AFM [0001] ₄ ^A	157	93	233	0.97	0.90	1.01	0.25	1.69	1.63
	AFM [0001] ₂ ^A	153	88	221	0.99	0.80	0.92	0.26	1.74	1.70
	FM	155	94	235	0.91	0.78	1.12	0.25	1.65	1.49
	NM	180	50	136	1.46	1.06	3.23	0.37	3.60	2.86

^aReference 39.

^bDerived from equations in this work, but with data from Ref. 39.

^cReference 30.

TABLE IV. Upper and lower experimental values of B (GPa), G (GPa), and E (GPa) for $M_2\text{GaC}$ phases, compared to the values of the moduli for AFM $[0001]_4$ Mn_2GaC from Table III.

	B (experiment)	G (experiment)	E (experiment)
Highest	251 (Ta_2AlC) ^a	125 (Ti_2SC) ^b	294 (Nb_2AlC) ^c
Lowest	127 (Zr_2InC) ^d	80 (Cr_2GeC) ^e	178 (Zr_2SnC) ^f
	B_V	G_V	E
Mn_2GaC	157	93	233

^aReference 43.

^bReference 45.

^cReference 47.

^dReference 44.

^eReference 46.

^fReference 48.

$$A_{s2} = \frac{2C_{44}}{C_{11} - C_{12}}. \quad (8)$$

For a perfectly isotropic material, $A_{c,s1,s2} = 1$. For Mn_2GaC , $A_c \sim 0.97$, $A_{s1} \sim 0.9$, and $A_{s2} \sim 1$, which indicates that the phase is close to being elastically isotropic, in line with what has been experimentally confirmed for a number of MAX phases.⁴² The results further suggest that Mn_2GaC is more elastically isotropic than both Ti_2GaC and V_2GaC , and approximately as isotropic as in-AFM1 Cr_2GaC .

Mn_2GaC possesses the highest Poisson's ratio out of all four $M_2\text{GaC}$ phases included in this work, $\nu = 0.25$, which is also a fairly high number as compared to many other MAX phases; common ratios derived from experimental measurements are 0.16 – 0.2, with Cr_2GeC as at least one outlier ($\nu = 0.29$).^{42,46} Here, we have calculated ν using the relation

$$\nu = \frac{3B_V - 2G_V}{2(3B_V + G_V)}. \quad (9)$$

As measurements of the machinability, we use the Pugh ductility index μ_D which is defined as the bulk – to – shear modulus ratio,⁵⁰ and the machinability index μ_M , which is given by B/C_{44} .⁵¹ Compared to the other $M_2\text{GaC}$ phases, Mn_2GaC has the highest value of both μ_D and μ_M : 1.69 and 1.63, respectively. This can be attributed to the high shearability (C_{44} is related to shear as well) of Mn_2GaC , since its bulk modulus is comparatively low, as discussed above.

For the $M_2\text{GaC}$ phases, the only reported experimental data are on the bulk modulus of Cr_2GaC . However, with the exception of the elastic constants C_{ij} , quite a lot of experimental data can be found for $M_2\text{AC}$ phases with A elements other than Ga. In Ref. 42, for instance, the experimental bulk, shear, and Young's moduli for Ti_2AC ($A = \text{Al}, \text{S}$), V_2AC ($A = \text{Al}$), Cr_2AC ($A = \text{Al}, \text{Ge}$), Nb_2AC ($A = \text{Al}$), and Ta_2AC ($A = \text{Al}$) are listed and compared to theoretical data. This comparison shows that theory tends to overestimate G and E, and either under or overestimate B. The differences between theory and experiment are largest for Ti_2GeC ($\sim 32\%$ for B from diamond anvil cell measurements) and Cr_2AlC ($\sim 25\%$ for G and E). These differences may be explained by theoretical approximations, such as calculations being mostly performed at 0 K and on crystals without impurities or vacancies, and on measurement artefacts.

FIG. 7. Theoretical and experimental values of the elastic moduli for $M_2\text{AlC}$ and $M_2\text{GaC}$.

In Figs. 7(a)–7(c), we compare our theoretical ground state values of the Voigt bulk, Voigt shear, and Young's moduli for the four $M_2\text{GaC}$ phases listed in Table III to theoretical and experimental moduli for the corresponding $M_2\text{AlC}$ phases (also calculated in this work). Since the predicted trends for $M_2\text{GaC}$ closely follow those for the theoretical $M_2\text{AlC}$ moduli, which in turn lie reasonably close to the experimental values, we suggest that the experimental $M_2\text{GaC}$ moduli should follow similar trends as, and be close in magnitude to, the $M_2\text{AlC}$ ones. The latter hypothesis is partly supported by a comparison of the magnitude of the experimental bulk modulus of Cr_2AlC found in Ref. 43 to that of Cr_2GaC in Ref. 52: the diamond anvil cell measurements yield a difference of ~ 25 GPa (note that Refs. 53 and 54 instead use velocity of sound measurements to determine the bulk moduli—hence the different results).

IV. CONCLUSIONS

We have investigated the recently discovered magnetic MAX phase Mn_2GaC by means of first – principles calculations. The 0 K ground state magnetic configuration, which is predicted to be antiferromagnetic, is thermodynamically stable with respect to the set of most competing phases as well

as stable with respect to lattice vibrations and structural distortions.

The electronic band structure indicates possible anisotropic conductive properties, and that the density of states is depending on the magnetic state, and whether the Mn spin configuration changes orientation upon crossing the Ga layers. A similar redistribution was also seen for the phonon density of states.

From calculations of the five elastic constants C_{ij} , we have determined the Voigt bulk modulus B_V , the Voigt shear modulus G_V , and the Young's modulus E of Mn_2GaC to be 157, 93, and 233 GPa, respectively. We further determined the Poisson's ratio ν , and the machinability indices μ_D and μ_M to be 0.25, 1.69, and 1.63. Three anisotropy factors were also calculated: the compression anisotropy factor A_s , and two different shear anisotropy factors A_{s1} and A_{s2} , with magnitude 0.97, 0.90, 1.01, respectively. This suggests that Mn_2GaC is relatively elastically isotropic.

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