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N.B.: When citing this work, cite the original publication.

Chaix-Pluchery, O., Thore, A., Kota, S., Halim, J., Hu, C., Rosén, J., Ouisse, T., Barsoum, M. W., (2017), First-order Raman scattering in three-layered Mo-based ternaries: MoAlB, Mo₂Ga₂C and Mo₂GaC, *Journal of Raman Spectroscopy*, 48(5), 631-638. <https://dx.doi.org/10.1002/jrs.5087>

Original publication available at:

<https://dx.doi.org/10.1002/jrs.5087>

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First-order Raman Scattering in Three Layered Mo-based Ternaries: MoAlB, Mo₂Ga₂C and Mo₂GaC

By

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Abstract

Here we report, for the first time, on the first-order Raman spectra of the layered Mo-based ternaries: MoAlB, Mo₂Ga₂C and Mo₂GaC. Polycrystalline samples were fabricated and well-defined Raman spectra were recorded. When the experimental peak positions were compared with those predicted from density functional theory, good agreement was obtained, indirectly validating both. Furthermore, all modes in the three compounds were symmetry assigned.

Keywords: MoAlB, Mo₂Ga₂C, MoGaC, Raman scattering, DFT calculations

Introduction

The ternary nanolaminated transition metal carbides and nitrides, known as the MAX phases, have been studied extensively over the last two decades due to their unusual combination of metallic and ceramic-like physical properties. These include relatively high elastic stiffness, high electronic and thermal conductivity, thermal shock resistance, machinability. Several of the MAX phases are also creep, oxidation, and corrosion resistant, which makes them promising candidates for high-temperature structural components. In the search for other unique nanolaminated compounds, several MAX phase-like carbides (e.g. Zr₃Al₃C₅ ^[1], Mo₂Ga₂C ^[2]) and ternary transition metal borides are among those that have recently drawn interest ^[3,4].

Mo₂GaC exhibits the usual hexagonal structure of MAX phases (space group *P6₃/mmc* or *D_{6h}* ^[4]) with two formula units per unit cell; Mo₂Ga₂C exhibits the same hexagonal structure and only differs from Mo₂GaC by having two Ga layers instead of one in between Mo₂C layers (Fig. 1(a, b)) ^[2,5]. In Mo₂Ga₂C, the Mo and Ga atoms lie on 4f sites and C atoms on 2a

sites. In Mo_2GaC , as in all the 211 MAX phases, the Mo, Ga and C atoms occupy 4f, 2d and 2a sites, respectively. In both cases, CMo_6 edge-sharing octahedra are separated by one or two layers of Ga atoms. It is worth noting here that the two layers of Ga are stacked one on top of the other, viz. in a simple cubic arrangement.

Among the nanolaminated ternary transition metal borides, we have recently shown that MoAlB is a highly oxidation resistant compound containing edge-sharing Mo-B trigonal prisms with two interleaving planar layers of Al atoms (Fig. 1(c)) [6, 7]. Insofar as the anisotropic bonding between the transition metal-carbon and transition metal-A layer is responsible for the unique physical properties of the MAX phases, a detailed study of Mo_2GaC , $\text{Mo}_2\text{Ga}_2\text{C}$ and MoAlB should allow us to better assess the effects of stoichiometry, chemistry, and structure on their vibrational behaviour.

The experimental and theoretical Raman scattering of several 211 MAX phases, like Mo_2GaC have been investigated in previous studies [8-15]. For the 211 MAX phases, four first-order Raman active optical modes are present ($A_{1g} + E_{1g} + 2E_{2g}$) and are due to the vibrations of only the M and A elements (see below). Given the identical Mo-C sublattices of Mo_2GaC and $\text{Mo}_2\text{Ga}_2\text{C}$, one might expect similar modes and additional ones arising from shear or longitudinal vibrations of the planar Ga bilayer in $\text{Mo}_2\text{Ga}_2\text{C}$, as indeed observed.

The present paper reports, for the first time, on the Raman scattering, coupled with density functional theory calculations, of the vibrational spectrum of MoAlB , $\text{Mo}_2\text{Ga}_2\text{C}$ and Mo_2GaC . To the best of our knowledge, Raman spectra of such Mo-containing compounds are not reported in literature and thus among other aims, this study aims to provide reference data for future Raman investigations of these compounds in the bulk or thin film state.

Experimental Details

Synthesis

Powders of MoAlB and Mo_2GaC were synthesized according to previous reports [7, 16]. Powders of $\text{Mo}_2\text{Ga}_2\text{C}$ were synthesized by a reaction between Mo_2C powders (Alfa Aesar, Ward Hill, MA, -325 mesh, 99.5 % pure) and Ga (Alfa Aesar, Ward Hill, MA, 99.5 wt% purity). The powders were mixed in a 1:8 molar ratio and placed in a quartz tube that was evacuated using a mechanical vacuum pump and sealed. The latter was placed in a horizontal tube furnace that was heated at a rate of $10\text{ }^\circ\text{C min}^{-1}$ to $850\text{ }^\circ\text{C}$, and held at that temperature for 48 h. After passively cooling in the furnace, the lightly sintered material was crushed, using a mortar and pestle, and returned back to the quartz tube. The latter was evacuated, sealed, and re-heated at a rate of $10\text{ }^\circ\text{C min}^{-1}$ to $850\text{ }^\circ\text{C}$ and held at temperature for an extra

456 h. Rietveld refinement of the XRD patterns for $\text{Mo}_2\text{Ga}_2\text{C}$ (not shown) indicated that < 5 wt. % binary Mo_2C was present in the powders as a secondary phase. All three powders were uniaxially cold-pressed into polycrystalline pellets under a load corresponding to 300 MPa, for further analysis.

Characterization

X-ray diffraction (XRD) measurements were performed with a Bruker D8 Advance diffractometer in a $\theta/2\theta$ configuration using the $\text{CuK}\alpha_1$ radiation ($\lambda = 1.540598$ nm). Raman spectra from the polycrystalline pellets were recorded using a Jobin Yvon/Horiba Labram spectrometer equipped with a liquid nitrogen cooled charge-coupled device detector. The experiments were conducted in the micro-Raman mode at room temperature. An Ar^+ laser radiation (514.5 nm and 488 nm) was focused to a spot size $\sim 1 \mu\text{m}^2$ on the sample surface with an incident power between 0.35 and 1.2 mW, depending on the sample and exciting line. Raman spectra were calibrated using a silicon reference spectrum at room temperature.

DFT calculations

The structural relaxations of the unit cells were performed using density functional theory (DFT) as implemented in the Vienna Ab initio Simulation Package (VASP) code ^[17-20], together with the projector augmented wave method ^[21]. The generalized gradient approximation developed by Perdew, Burke, and Ernzerhof (PBE-GGA) was used to model the exchange-correlation potential ^[22]. The convergence criterion with respect to the total energy of each compound was set to 0.1 meV/atom; the plane wave cutoff energy in all calculations carried out in this work was 400 eV.

To obtain the vibrational properties, the finite displacement supercell method was utilized. The atomic displacements in the supercells were created with the PHONOPY software package ^[23, 24], and the dynamical matrix containing the force constants was then calculated using VASP-DFT with the PBE-GGA. For MoAlB , sufficient convergence with respect to the force constants was reached for a $2 \times 2 \times 1$ supercell and a $10 \times 10 \times 10$ Monkhorst-Pack k-point grid, while for both $\text{Mo}_2\text{Ga}_2\text{C}$ and Mo_2GaC , it was reached for a $3 \times 3 \times 1$ supercell and $5 \times 5 \times 3$ k-point grid. The calculations of the vibrational frequencies and the assignments of irreducible representation labels were done with PHONOPY.

Results and discussion

Structural characterization of MoAlB , $\text{Mo}_2\text{Ga}_2\text{C}$ and Mo_2GaC samples

XRD patterns of the three samples are shown in Fig. 2. With the exception of three very weak lines at 36.28, 41.95 and 56 °2 θ assigned to MoAl₅ (ICDD file n°00-044-1101), all other peaks shown in the XRD pattern of MoAlB (Fig. 2(a)) have been indexed and belong to MoAlB (ICCD file n° 01-072-1277).

Except for seven weak lines assigned to Mo₂C (ICDD file n°00-035-0787), all other peaks shown in the XRD pattern of Mo₂Ga₂C (Fig. 2(b)) have been directly compared to that given in Ref. [2] through a file created with the Topas software V4.2 from Bruker. The match is excellent [2]. We note that the high intensity of the (00*l*) reflections, especially (008), clearly reveals a strong preferred orientation along the c-axis of the Mo₂Ga₂C pellet, which is quite common for MAX phases. Lastly, the most intense peaks in the XRD pattern of Mo₂GaC (Fig. 2(c)) can be easily indexed to Mo₂GaC (ICCD file n°04-005-0051), but only after a little adjustment of the lattice parameters probably due to a slight non-stoichiometry of the sample. Herein the following lattice parameters have been obtained $a = b = 3.037 \text{ \AA}$, $c = 13.191 \text{ \AA}$ instead of $a = b = 3.017 \text{ \AA}$, $c = 13.180 \text{ \AA}$ which are reference values. In addition to some weak Mo₂C lines, two weak lines of graphite are also visible, as well as, a non-identified weak line at 37.28 °2 θ .

Vibrational analysis at the zone center and Raman spectra

Vibrational analysis

MoAlB exhibits an orthorhombic structure (space group *Cmcm* or *D*_{2h}¹⁷) with two formula units per unit cell and all the atoms in special positions 4c [4]. Figure 3(a) shows the calculated phonon dispersion curves and the vibrational density of states. The states between 0 and ~12.5 THz (~ 412.5 cm⁻¹) are mainly occupied by Mo and Al vibrations, with a tendency for the significantly heavier Mo atoms to dominate the lower end of this range. Above 12.5 THz, the states are almost exclusively occupied by vibrations of the light B atoms, which is analogous to what occurs in the MAX phases [25].

The six atoms of the primitive cell of MoAlB give rise to 18 zone center vibrational modes, 15 of them are optical modes and three are acoustic modes. According to the factor group analysis at the Γ point [26, 27], the irreducible representations for the optical modes can be expressed as

$$\Gamma_{\text{opt}} = 3A_g + 3B_{1g} + 3B_{3g} + 2B_{1u} + 2B_{2u} + 2B_{3u}$$

where A_g , B_{1g} , B_{3g} are Raman-active modes and B_{1u} , B_{2u} , B_{3u} are IR-active modes. A schematic representation of the Raman-active modes of MoAlB is shown in Fig. 4(a).

The calculated phonon dispersion curves and vibrational density of states in Mo₂Ga₂C are shown in Fig. 3(b), the corresponding ones for Mo₂GaC in Fig. 3(c). In both Mo-Ga-C

compounds, the states in the lower half of the frequency range, i.e., 0-10 THz (= 0-330 cm⁻¹), are dominated by the Mo and Ga vibrations, while vibrations of the light C atoms, just as for B in MoAlB, dominate the states in the upper half. The DOS of Mo₂Ga₂C differs from that of Mo₂GaC mainly in that its total number of Ga states is greater and that it exhibits a slight shift of the Mo states towards higher vibrational frequencies.

The ten atoms in the primitive cell of Mo₂Ga₂C lead to 27 optical modes, expressed as

$$\Gamma_{\text{opt}} = 2A_{1g} + 2B_{1g} + 2E_{1g} + 2E_{2g} + 2A_{2u} + 3B_{2u} + 2E_{1u} + 3E_{2u},$$

whereas the eight atoms in the primitive cell of Mo₂GaC give rise to 21 optical modes, expressed as

$$\Gamma_{\text{opt}} = A_{1g} + 2B_{1g} + E_{1g} + 2E_{2g} + 2A_{2u} + 2B_{2u} + 2E_{1u} + 2E_{2u}$$

Among the optical modes of both compounds, A_{1g}, E_{1g}, E_{2g} are Raman-active modes, A_{2u}, E_{1u} are IR-active modes and the remaining B_{1g}, B_{2u} and E_{2u} are silent. It is to be noted that vibrational modes coming from the C atoms only give rise to IR-active or silent modes and have no contribution to the Raman spectrum. This is seen for Mo₂Ga₂C in Fig. 4(b), which shows the atomic displacements of the Raman-active modes. The modes for the 211 MAX phase, Mo₂GaC, are reproduced from Ref. [11, 12] in Fig. 4(c).

Thus, nine lines are expected in the Raman spectrum of MoAlB (3A_g+3B_{1g}+3B_{3g}), six lines for Mo₂Ga₂C (2A_{1g}+2E_{1g}+2E_{2g}) and four lines for Mo₂GaC (A_{1g}+E_{1g}+2E_{2g}).

Raman Spectra

The Raman spectra of the three compositions measured herein are reported in Fig. 5. The Raman spectrum of the MoAlB sample (Fig. 5(a)) shows ten Raman lines while nine modes are expected from the vibrational analysis; the first three peaks are well-defined lines, whereas weak lines are observed above 300 cm⁻¹. The comparison between observed and calculated positions in Table 1 first allows the identification of the unexpected tenth line: it occurs around 495 cm⁻¹ and partially overlaps the line at 463 cm⁻¹ (see inset in Fig. 5(a)). This line could not be assigned. The comparison also indicates good agreement between experimental and calculated values, with the experimental ones being systematically higher (maximum difference = +8 cm⁻¹), and allows all the nine Raman modes to be symmetry assigned.

Before delving in the details of the Mo₂Ga₂C and Mo₂GaC spectra, we note that the spectra measured on different points of the samples revealed the presence of gallium oxide and carbon in both samples and some mixtures of both phases, especially in Mo₂GaC. The

spectrum of β -Ga₂O₃ (monoclinic structure, space group $C2/m$ or C_{2h}^3), being sometimes of high intensity, was easily identified from spectra given in Ref. [28], in particular due to its very strong A_g mode at ~ 201 cm⁻¹. When present in the samples, this phase was found simultaneously with graphite-type carbon (characteristic lines at 1355-1357 and 1585-1601 cm⁻¹). Despite the presence of these additional phases, Raman spectra of both compounds were recorded and their Raman modes identified from the calculated spectra.

The Mo₂Ga₂C Raman spectrum is shown in Fig. 5(b). Only five well-defined lines are observed compared to the six expected ones. The symmetry assignment has been made from the comparison with the calculated modes, as shown in Table 1. It can be observed first that the line measured at 179 cm⁻¹ can be indifferently assigned to E_{2g}(2) and E_{1g}(2) modes calculated at 181 and 182 cm⁻¹, respectively. Thus, all the expected modes are observed and a good agreement is obtained between calculated and observed positions of the first five modes, the difference being greatest for the last one (14 cm⁻¹).

In general, the Raman signal of the Mo₂GaC sample was weak regardless of the exciting wavelength. This led us to record a large number of spectra under different conditions of laser power and wavelengths including 488 nm, 514.5 nm and 682.8 nm (not shown) in order to identify the four Mo₂GaC Raman lines with certainty. The spectra shown in Fig. 5(c) are some of the best obtained with the 488 nm (bottom, blue) and 514.5 nm (top red) lasers. As seen in Fig. 5(c), the lines at 77 and 312 cm⁻¹ belong to Mo₂Ga₂C; those at 208 cm⁻¹ to β -Ga₂O₃. The four remaining lines, occurring in all measured spectra, can be attributed with certainty to Mo₂GaC: the first one at 98 cm⁻¹ (E_{2g}(1) mode) is the only well-defined line; the other ones fluctuate slightly in wavenumbers from one spectrum to another and, as a consequence, the experimental positions reported in Table 1 are those of the best defined lines, i.e. 158, 172 and 252 cm⁻¹, respectively assigned to E_{1g}, E_{2g}(2) and A_{1g}. Good agreement is observed between the experimental and calculated positions of the two E_{2g} modes; the agreement is less good for the E_{1g} and A_{1g} modes and can be explained by the difficulty of recording good, strong peaks. Here the peak at 158 cm⁻¹ is weak in intensity; the one at 252 cm⁻¹ is quite broad, probably due to the overlap with the A_{1g}(1) mode of Mo₂Ga₂C at 234 cm⁻¹.

At this stage it is instructive to critically analyze the spectra obtained in light of what is known about the structures and bonding in these solids. First we compare Mo₂GaC and Mo₂Ga₂C. They both possess the hexagonal structure ($P6_3/mmc$); the only structural difference being the insertion of an additional Ga layer in Mo₂Ga₂C. Comparing the atomic

displacements associated to Raman modes in $\text{Mo}_2\text{Ga}_2\text{C}$ (Fig. 4(b)) and Mo_2GaC (Fig. 4(c)), it is clear that the following similarities are noteworthy. More specifically:

- i) The first mode, $E_{2g}(\omega_1)$, involves parallel shear displacements of Mo and Ga atoms within the basal plane, the only difference being the motion of two Mo atoms in $\text{Mo}_2\text{Ga}_2\text{C}$ ($\omega_{\text{exp}} = 67 \text{ cm}^{-1}$) instead of one in Mo_2GaC ($\omega_{\text{exp}} = 98 \text{ cm}^{-1}$). Neglecting the small oscillations of the Mo atoms in the $E_{2g}(\omega_1)$ mode of $\text{Mo}_2\text{Ga}_2\text{C}$ (Fig. 4(b)), the coupled Ga atoms do not move with respect to one another, making the mode equivalent to the $E_{2g}(\omega_1)$ mode of Mo_2GaC (Fig. 4(c)) but with a doubled oscillating mass. The ratio between the two wavenumbers should thus simply be $\sqrt{2}$, which is almost exactly found, both theoretically and experimentally (Table 1). This is an important result since it is a totally independent check on the validity of our analysis, be it theoretical or experimental. We note in passing that these shear modes are some of the lowest ever recorded for the MAX phases.
- ii) The second close modes are $E_{1g}(\omega_4)$ in $\text{Mo}_2\text{Ga}_2\text{C}$ ($\omega_{\text{exp}} = 179 \text{ cm}^{-1}$) and E_{1g} in Mo_2GaC ($\omega_{\text{exp}} = 158 \text{ cm}^{-1}$); both involve anti-parallel shear displacements of Mo atoms only. Each mode can be directly associated to another mode in each compound, only differing by parallel instead of anti-parallel shear displacements of the Mo atoms: $E_{2g}(\omega_3)$ in $\text{Mo}_2\text{Ga}_2\text{C}$ ($\omega_{\text{exp}} = 179 \text{ cm}^{-1}$), $E_{2g}(2)$ in Mo_2GaC ($\omega_{\text{exp}} = 172 \text{ cm}^{-1}$) which also involves small displacements of the Ga atoms. The four modes should lead to almost equal wavenumbers since the Mo planes vibrate almost independently and have similar local environments, with almost immobile or slightly oscillating Ga atoms (Fig. 4(b) and 4(c)). This is indeed found theoretically for both compounds ($\omega_{\text{calc}} = 181 \text{ cm}^{-1}$ for both E_{2g} modes, and 182 and 178 cm^{-1} for E_{1g} modes in $\text{Mo}_2\text{Ga}_2\text{C}$ and Mo_2GaC , respectively (Table 1) and experimentally for $\text{Mo}_2\text{Ga}_2\text{C}$ ($\omega_{\text{exp}} = 179 \text{ cm}^{-1}$ for both modes).
- iii) A noticeable discrepancy exists with the experimental values of E_{1g} ($\omega_{\text{exp}} = 158 \text{ cm}^{-1}$) and $E_{2g}(2)$ ($\omega_{\text{exp}} = 172 \text{ cm}^{-1}$) in Mo_2GaC which might be partly due to a very weak intensity in the case of the E_{1g} rendering an accurate determination of the line positions difficult (see Fig. (5)).
- iv) The A_{1g} mode in Mo_2GaC ($\omega_{\text{exp}} = 252\text{-}255 \text{ cm}^{-1}$) is associated to anti-symmetrical longitudinal displacements along the c-axis of the Mo atoms, whereas the corresponding $A_{1g}(\omega_5)$ mode in $\text{Mo}_2\text{Ga}_2\text{C}$ ($\omega_{\text{exp}} = 234 \text{ cm}^{-1}$) involves the same displacements of the Mo and Ga atoms, thus increasing the distance between the Mo layers. It is thus not surprising that these modes are close in energy.

v) The $E_{1g}(\omega_2)$ ($\omega_{\text{exp}} = 78 \text{ cm}^{-1}$) and $A_{1g}(\omega_6)$ ($\omega_{\text{exp}}=317 \text{ cm}^{-1}$) modes in $\text{Mo}_2\text{Ga}_2\text{C}$ are associated to vibrations involving the planar Ga bilayer and have no equivalent in Mo_2GaC . The internal consistency between these two different compounds and their modes is gratifying and are important indicators that both theory and experiment are valid.

Along the same lines it is instructive to compare $\text{Mo}_2\text{Ga}_2\text{C}$ and MoAlB . And while they differ by their crystal structure (hexagonal - $P6_3/mmc$ vs. orthorhombic - $Cmcm$, respectively) both are layered compounds with two Ga layers along the c-axis and two Al layers along the b-axis, respectively. As for the comparison between modes in these compounds from the schematics shown in Fig. 4, only one mode appears to involve the same atoms vibrating along the same directions: viz. $A_g(\omega_3)$ in MoAlB ($\omega_{\text{exp}} = 260 \text{ cm}^{-1}$) and $A_{1g}(\omega_5)$ in $\text{Mo}_2\text{Ga}_2\text{C}$ ($\omega_{\text{exp}} = 234 \text{ cm}^{-1}$). They both involve anti-symmetrical longitudinal displacements of the Mo and Ga atoms along the c-axis in $\text{Mo}_2\text{Ga}_2\text{C}$, of the Mo and Al atoms along the y-axis in MoAlB , increasing the distance between the two Al- and two Ga layers, respectively. The fact that these modes are close in energy is thus expected.

Lastly, two open questions remain from XRD and Raman analyses of the $\text{Mo}_2\text{Ga}_2\text{C}$ and Mo_2GaC samples: i) Mo_2C has been detected in the X-ray patterns of both samples but not in their Raman spectra; ii) $\beta\text{-Ga}_2\text{O}_3$ has been often detected in both samples by Raman spectroscopy but not in the X-ray patterns. The second point can be explained if the oxide is present very locally in the samples since Raman spectroscopy is a local probe; it is the case for the detection of $\text{Mo}_2\text{Ga}_2\text{C}$ in the Mo_2GaC sample (the reverse is also found but not often). The $\beta\text{-Ga}_2\text{O}_3$ could also be amorphous. Concerning the first point, all the Raman lines have been assigned in all spectra of both samples, i.e. there is no non-assigned line which could come from Mo_2C .

Summary and conclusions

The investigation of MoAlB , $\text{Mo}_2\text{Ga}_2\text{C}$ and Mo_2GaC polycrystalline samples by Raman scattering is reported for the first time. In all cases, well-defined spectra were recorded and all Raman modes predicted by the selection rules have been measured. DFT calculations of their theoretical vibrational spectra have been performed and a good agreement between experimental and calculated positions is observed for most lines allowing the symmetry assignment of all Raman modes in the three compounds. This study will allow these Raman spectra to be used as reference data for future Raman investigations on these Mo-containing materials in the bulk or thin film state.

Acknowledgements

H. Roussel, LMGP Grenoble, is acknowledged for his assistance in the X-ray diffraction experiments. The calculations were carried out using supercomputer resources provided by the Swedish National Infrastructure for Computing (SNIC) at the PDC Center for High Performance Computing, and the National Supercomputer Centre (NSC). We also acknowledge the support from the Swedish Research Council through Project Grants 621-2011-4420 and 621-2014-4890 the Swedish Foundation for Strategic Research through the Synergy Grant FUNCASE Functional Carbides for Advanced Surface Engineering.

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Figure captions

Figure 1: Crystal structures of (a) Mo_2GaC , (b) $\text{Mo}_2\text{Ga}_2\text{C}$ and (c) MoAlB , showing atoms of Mo (purple), C (black), Ga (green), B (pink) and Al (blue).

Figure 2: XRD patterns of (a) MoAlB , (b) $\text{Mo}_2\text{Ga}_2\text{C}$ and (c) Mo_2GaC polycrystalline samples. For clarity, only the more intense diffraction peaks related to the three compounds are indexed, the weaker peaks being pointed out with vertical dashes.

Figure 3: Phonon dispersion curves and density of states of (a) MoAlB , (b) $\text{Mo}_2\text{Ga}_2\text{C}$ and (c) Mo_2GaC .

Figure 4: Schematic of the Raman active modes of (a) MoAlB , (b) $\text{Mo}_2\text{Ga}_2\text{C}$ and (c) Mo_2GaC . In order to show the three B_{3g} modes in MoAlB , the unit cells have been rotated 90° clockwise into the plane of the paper, relative to the unit cells of the six other modes.

Figure 5: Raman spectra of (a) MoAlB , (b) $\text{Mo}_2\text{Ga}_2\text{C}$ and (c) Mo_2GaC polycrystalline samples recorded at room temperature with the 514.5 nm (a, b, c) and the 488 nm (c) excitation lines of an Ar^+ laser. An enlargement of the MoAlB spectrum above 300 cm^{-1} is shown in the inset of (a).

Table 1: Calculated, ω_{calc} and experimentally observed, ω_{exp} positions, in cm^{-1} , and symmetry assignments of the Raman modes in MoAlB, Mo₂Ga₂C and Mo₂GaC polycrystalline samples.

MoAlB (<i>Cmcm</i>)			Mo₂Ga₂C (<i>P6₃/mmc</i>)			Mo₂GaC (<i>P6₃/mmc</i>)		
Mode symmetry	ω_{calc} (cm^{-1})	ω_{exp} (cm^{-1})	Mode symmetry	ω_{calc} (cm^{-1})	ω_{exp} (cm^{-1})	Mode symmetry	ω_{calc} (cm^{-1})	ω_{exp} (cm^{-1})
B _{1g} (1)	171	175	E _{2g} (1)	68	67	E _{2g} (1)	96	98
B _{3g} (1)	203	206	E _{1g} (1)	71	78	E _{1g}	178	158
A _g (1)	252	260	E _{2g} (2)	181	179	E _{2g} (2)	181	172
B _{3g} (2)	330	332	E _{1g} (2)	182	179	A _{1g}	244	252
B _{1g} (2)	346	351	A _{1g} (1)	230	234			
A _g (2)	400	406	A _{1g} (2)	303	317			
B _{1g} (3)	455	463						
A _g (3)	626	629						
B _{3g} (3)	751	755						

Mo_2GaC

(a)

$\text{Mo}_2\text{Ga}_2\text{C}$

(b)

MoAlB

(c)

(a)

(b)

(c)