Comparative study of Mo_2Ga_2C with superconducting MAX phase Mo_2GaC: First-principles calculations

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The structural, electronic, optical and thermodynamic properties of Mo_2Ga_2C are investigated using density functional theory (DFT) within the generalized gradient approximation (GGA). The optimized crystal structure is obtained and the lattice parameters are compared with available experimental data. The electronic density of states (DOS) is calculated and analyzed. The metallic behavior for the compound is confirmed and the value of DOS at Fermi level is 4.2 states per unit cell per eV. Technologically important optical parameters (e.g., dielectric function, refractive index, absorption coefficient, photo conductivity, reflectivity, and loss function) are calculated for the first time. The study of dielectric constant (ε_1) indicates the Drude-like behavior. The absorption and conductivity spectra suggest that the compound is metallic. The reflectance spectrum shows that this compound has the potential to be used as a solar reflector. The thermodynamic properties such as the temperature and pressure dependent bulk modulus, Debye temperature, specific heats, and thermal expansion coefficient of Mo_2Ga_2C *MAX* phase are derived from the quasi-harmonic Debye model with phononic effect also for the first time. Analysis of T_c expression using available parameter values (DOS, Debye temperature, atomic mass, etc.) suggests that the compound is less likely to be superconductor.

Keywords: first-principles calculations, density of states (DOS), optical properties, thermodynamic properties

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1. Introduction

Recently, the scientific community has paid significant attention to an unusual class of layered ternary carbide and nitride, the so-called *MAX* phases, because of their outstanding combination of properties, some of which are like ceramics and the others metallic.[1,2] To be specific, the properties with which a metal is applicable on an industrial scale are the machinability, damage tolarance, thermal and electrical conductivity, which are possessed by these materials. They also possess the properties of ceramics such as high elastic stiffness, refractory nature, and resistant to high-temperature oxidation.[3] The outstanding combination of these properties makes them attractive for potential applications in diverse fields from defense materials to electronic devices such as in defense, aerospace, automobiles, medical application, nuclear reactors and portable electronic devices where they are already used. The charismatic uniqueness of the *MAX* phases is motivating numerous research studies to expect that they can open the way to practical commercial applications for these materials in the future. So far, more than 70 different *MAX* phases have been experimentally synthesized[4] and also a good number of *MAX* phases have been theoretically predicted. The research in searching the new *MAX* phases is growing fast in order to discover more new *MAX* phase compounds due to their properties mentioned above. The M_2AX (211) phases including solid solutions with M = Ti, V, Cr, Nb, Ta, Zr, Hf, A = Al, S, Sn, As, In, Ga, and X = N, C, have been studied extensively both experimentally and theoretically[5–11] (Refs. [1]–[29] in Ref. [5]). Among them, Mo_2GaC[12] is an important *MAX* phase showing superconducting characteristics with T_c $\sim$ 4.0 K. Very recently, Hu *et al.*[13] reported on the discovery of a totally new ternary hexagonal Mo_2Ga_2C phase, a counterpart of superconducting Mo_2GaC, which is assumed to be the first member of a distinct large family closely related to the *MAX* phases.

Studies of Mo_2Ga_2C phase have been reported in the literature. The structural and compositional analysis has been addressed by Lai *et al.*[14] Elastic and electronic properties have been investigated by Hadi.[15] Another plausible metastable structure with close-packed Ga layers is predicted from density functional calculations by Wang *et al.*[16] However, though structural, elastic and electronic properties were studied, the thermodynamic and optical properties were not taken into account. Moreover, due to the similarity of structure and electronic bonding to those of superconducting Mo_2GaC, Mo_2Ga_2C might also be a superconductor. The possibility of this property is not taken into consideration in the previous studies.

The thermodynamic properties are very important in solid state science and considered as the basis for industrial application of solids because material behavior can be obtained from thermodynamic properties under high temperatures and high pressure. Moreover, the optical properties provide the infor-

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mation about the electronic response of the materials which are related to the electronic properties of solids.[17] Therefore, an investigation of these properties is significantly necessary for fundamental physics and potential applications.

In this work, we aim to provide some additional information to the existing data on the physical properties of Mo_2Ga_2C phase by using the first-principles method, and we especially focus on the possible occurrences of superconductivity, thermodynamics, and optical properties.

2. Computational methods

The calculations were carried out by using the Cambridge Serial Total Energy Package (CASTEP) code[18] based on the density-functional theory.[19] The generalized gradient approximation (GGA) of Perdew–Burke–Ernzerhof (PBE) scheme[20] is used as the exchange and correlation function. The electrostatic interaction between valence electron and ionic core is represented by the ultrasoft pseudopotentials, and the cutoff energy for the plane wave expansion is 550 eV. A $17 \times 17 \times 3$ k-point mesh of Monkhorst–Pack[21] scheme was used for integration over the first Brillouin zone. The Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm[22] technique was applied to optimize the atomic configuration and density mixing is used to optimize the electronic structure.

3. Results and discussion

3.1. Structural properties

Like all the other *MAX* phases, the new compound Mo_2Ga_2C crystallizes in the hexagonal system with space group $P6_3/mmc$ (No. 194), and is not only similar in crystal system but also similar in unit cell structure to 211 *MAX* phase, such as the unit cell that contains two formula units. The number of atoms per unit cell is not the same. In the case of 211 *MAX* phase there are 8 atoms in their unit cell, whereas the new compound Mo_2Ga_2C has 10 atoms in its unit cell. There is a difference in the position of Ga atoms between Mo_2Ga_2C (4f Wyckoff position) and Mo_2GaC (2d Wyckoff position). The lattice constant a remains almost unchanged, but due to the extra Ga layer along the z-axis, lattice constant c is changed (Table 1). Figure 1 shows the unit cell structures of Mo_2Ga_2C and Mo_2GaC. Table 1 shows the lattice constants of Mo_2Ga_2C along with experimental data. Table 1 also contains the lattice constants of Mo_2GaC for comparison. The calculated lattice parameters are in reasonable agreement with the experimental results.

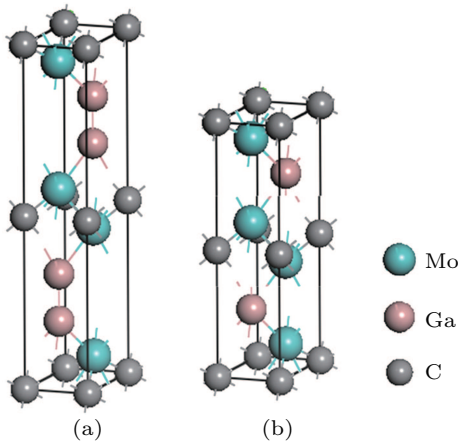


Fig. 1. (color online) Unit cell structures of (a) Mo_2Ga_2C and (b) Mo_2GaC.

Table 1. Lattice constants and atomic fractional coordinates of Mo_2Ga_2C and Mo_2GaC.

Phase	a/Å	c/Å	Ref.	Atomic position		
				Mo	Ga	C
Mo_2Ga_2C	3.047	18.164	This study	4f	4f	2a
	3.033	18.081	Expt.[13]			
	3.031	18.11	Expt.[14]			
	3.05374	18.13445	Theo.[15]			
Mo_2GaC	3.064	13.178	This study	4f	2d	2a
	3.01	13.18	Expt.[2]			

3.2. Electron DOS: possibility of superconductivity

Figure 2 shows the total and partial density of states (DOS) of (a) Mo_2Ga_2C and (b) Mo_2GaC. We use the DOS values to predict the possibility of superconductivity in Mo_2Ga_2C by comparing with that in Mo_2GaC. We also predict the possibilities of superconductivity in some materials by comparing with iso-structural superconducting phase in the same way.[23] The calculated DOS at the Fermi level for Mo_2Ga_2C is 4.2 states per unit cell per eV, whereas for Mo_2GaC it is found to be 4.5 states per unit cell per eV. It is significant to explain the nature of electrons close to the Fermi surface because these electrons will contribute to the formation of the superconducting state of materials. It is found that the DOS at the Fermi level originates mainly from Mo 5d states. In order to make clear the possible occurrence of superconductivity in Mo_2Ga_2C, the electron–phonon coupling properties of the compound should be investigated. The electron–phonon coupling can be expressed as $\lambda = N(E_F)V$, where V is the

degree of the inter-electron attractive interaction. Again, in McMillan's formula, T_c[24] is proportional to Debye temperature (θ_D) and an exponential term involving electron–phonon coupling constant, $\lambda = N(E_F)\langle I^2\rangle/M\langle\omega^2\rangle$. Here M is the relevant atomic mass, $\langle I^2\rangle$ the square of the e-phonon matrix element averaged over the Fermi surface, $\langle\omega^2\rangle$ is the relevant phonon frequency squared, and $N(E_F)$ is the DOS at E_F. This may be helpful for understanding the superconductivity of Mo_2Ga_2C. It can be seen from the expression that DOS would affect T_c only if the $\langle I^2\rangle$ values for Mo_2Ga_2C and Mo_2GaC are equal. The calculated values of θ_D are 471.2 and 483.8 K for Mo_2Ga_2C and Mo_2GaC,[15] respectively. The T_c equation when analyzed with all these factors of Mo_2Ga_2C and compared with superconducting Mo_2GaC indicates that the Mo_2Ga_2C compound is less likely to be superconductor. If the superconductivity in Mo_2Ga_2C will be confirmed in future, then the T_c value will also be expected to be very close to that of Mo_2GaC because T_c values for Mo_2Ga_2C and Mo_2GaC may be related to the phonon system. Indeed, for Mo_2Ga_2C and Mo_2GaC, the lattice parameter a, which determines the intra-atomic distances inside the conducting blocks, remains unchanged. This can lead to the same coupling constant λ. Definitely, these are assumptions, and to be sure about these assumptions the phonon spectra should be calculated. Finally, we note that the superconductivity for Mo_2Ga_2C has not been reported yet, the factors discussed here are compared with superconducting Mo_2GaC ($T_c \sim 4$ K), which allows us to assume the emergence of low-temperature superconductivity for Mo_2Ga_2C, and we believe that the relevant experiments will be of high interest.

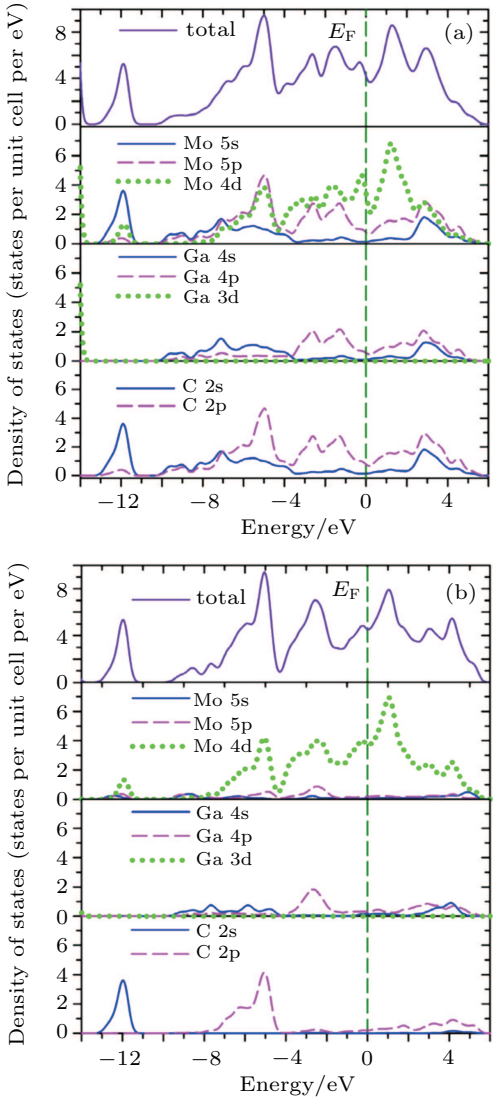


Fig. 2. (color online) Total and partial density of states (DOS) of (a) Mo_2Ga_2C and (b) Mo_2GaC.

3.3. Optical properties

Optical properties are used to describe the behaviors of materials subjected to electromagnetic radiation. In order to describe the response of Mo_2Ga_2C to electromagnetic radiation we calculate some important optical constants for the first time. The methods by which the optical constants are calculated can be found elsewhere.[23,25]

The optical constants of Mo_2Ga_2C for (100) polarization direction are shown in Fig. 3. To smear out the Fermi level for effective k-points on the Fermi surface, we used a 0.5 eV Gaussian smearing. When light of sufficient energy is incident onto a material, electrons are caused to transit from valence to conduction band. The electron transition takes part in making contributions to the optical properties of a metallike system, which affects mainly the low energy infrared part of the spectra. To calculate the dielectric function of metallic Mo_2Ga_2C, a Drude term with unscreened plasma frequency 3 eV and damping 0.05 eV is used.

The imaginary part, $\varepsilon_2(\omega)$ of the dielectric function $\varepsilon(\omega)$, dominates the electronic properties of crystalline material, which depicts the probability of photon absorption. The peaks of $\varepsilon_2(\omega)$ are associated with electron excitation. There is only one prominent peak around 2.0 eV (Fig. 3(b)). The large negative value of ε_1 is also observed in Fig. 3 (Fig. 3(a)) which is an indication of Drude-like behavior of metal. The refractive index is another technically important parameter for optical material in its technological applications in optical devices. The spectrum for refractive index n is demonstrated in Fig. 3(c). The static refractive index $n(0)$ is found to have a value of ~ 7 for Mo_2Ga_2C, while this value is 17.53 for Mo_2GaC.[26]

Figure 3(d) shows the absorption coefficient spectrum of Mo_2Ga_2C which reveals the metallic nature of the compound since the spectrum starts with non-zero value. Interestingly, a strong absorption coefficient is observed in the UV region. Moreover, the absorption coefficient is weak in the IR region but continuously increases toward the UV region, and reaches a maximum value at 7.7 eV. These results indicate that Mo_2Ga_2C is a promising absorbing material in the UV region.

A material with high absorption coefficient indicates that the absorption of photons is increased in the material, thereby exciting the electrons from the valence band to the conduction band. These materials are very important for optical and optoelectronic devices in the visible and ultraviolet energy regions. The band structure of the material shows no band gap, which indicates that the photoconductivity starts at zero photon energy as shown in Fig. 3(e). This type of photoconductivity confirms the good metallic nature of this compound. The reported absorption coefficient and photoconductivity spectrum of Mo_2GaC are almost the same as our results.[26]

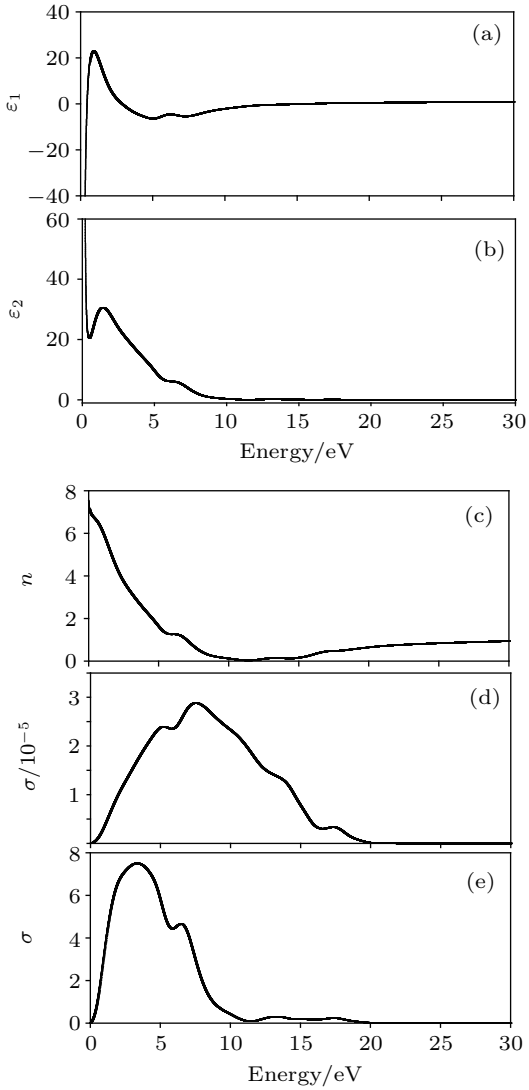


Fig. 3. (a) Real part and (b) imaginary part of dielectric constant, ε_1 and ε_2, respectively; (c) refractive index n, (d) absorption coefficients α, (e) conductivity σ of Mo_2Ga_2C.

The loss function $L(\omega)$, defined as the energy loss of an electron with high velocity passing through the material as shown in Fig. 4(a). In addition, the peaks in the $L(\omega)$ spectrum represent a plasma resonance property (a collective oscillation of the valence electrons). In our present case, the energy loss function curve is characterized by a peak which is known as the bulk plasma frequency ω_P and occurs at $\varepsilon_2 < 1$ and $\varepsilon_1 = 0$. In Fig. 4, the value of the effective plasma frequency ω_P is found to be ~ 16 eV, which is lower than that of Mo_2GaC (17.2 eV).[26] If the frequency of incident photon is greater than ω_P, then the material becomes transparent.

The reflectivity curve is also shown in Fig. 4(b). It is found that the reflectivity curve starts with a value of ~ 0.58 and exhibits no significant changes in the energy range up to ~ 6.0 eV, rises to a maximum value of ~ 0.9 at ~ 12 eV. Mo_2Ga_2C has roughly a similar reflectivity spectrum to those obtained by the other 211 and/or other *MAX* phases.[26] The value of reflectivity is always kept above 44%. Li *et al.*[27] reported Ti_3SiC_2, having an average reflectivity of $\sim 44\%$ in the visible light region, as a nonselective characteristic, which is responsible for solar heat reducing. Moreover, the reflectivity spectrum is steady and stable in a wide range (~ 6.0 eV) and then increases gradually. Therefore, it is expected that Mo_2Ga_2C compound is also appealing for the practical usage as a coating on spacecrafts to avoid solar heating. Moreover, the peak of loss function is associated with the trailing edges of the reflection spectrum. For example, the peak in $L(\omega)$ occurring at ~ 16 eV corresponds to an abrupt decrease in reflectivity.

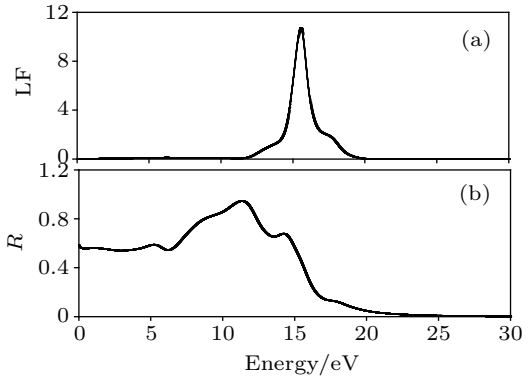


Fig. 4. (a) Loss function and (b) reflectivity of Mo_2Ga_2C.

3.4. Thermodynamic properties

The study of thermodynamic properties of materials permits a more in-depth understanding of the specific behavior of material under high temperature and pressure. The thermodynamic properties of Mo_2Ga_2C have been investigated by using quasi-harmonic Debye approximation.[28,29] The data calculated by using this method are in good agreement with experimental data proved by several authors.[30,31] The temperature- (0–1000 K) and pressure- (0–50 GPa) dependent polycrystalline aggregate properties including bulk modulus, Debye temperature, specific heats, and thermal expansion coefficients of Mo_2Ga_2C are calculated for the first time. The volume and total energy of Mo_2Ga_2C, calculated by the methodology described in Section 2, are used as input data in the Gibbs program. The method in which the volume and total energy are used as input in the Gibbs program can be found elsewhere.[32]

The bulk modulus, B at 0 GPa of Mo_2Ga_2C as a function of temperature is shown in Fig. 5(a); the inset represents B as a function of pressure. In the ambient condition, the B of Mo_2Ga_2C is lower than that of Mo_2GaC.[15] It can be found from the figure that the curve of B is nearly flat in a temperature range from 0 to 100 K. Above 100 K, B decreases slowly with temperatures up to 1000 K in a slightly nonlinear way. It is here noted that B is reduced by $\sim 5\%$ in a temperature range from 0 K to 1000 K. The value of B as a function of pressure at room temperature is shown in the inset. It is observed that B increases with increasing pressure at a given temperature and decreases with increasing temperature at a given pressure, because the effect of increasing pressure on material is similar to that of decreasing temperature of material, which means that the increase of temperature of the material leads to a reduction of its hardness. This phenomenon is well consistent with the trend of volume of the material although it is not shown in the figure.

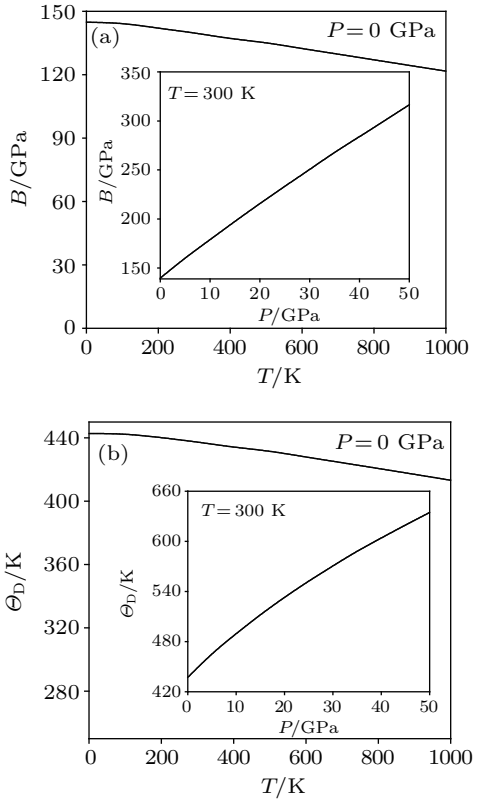


Fig. 5. Temperature-dependent (a) bulk modulus, B and (b) Debye temperature, Θ_D of Mo_2Ga_2C. The insets show pressure dependence.

Figure 5(b) displays the temperature dependence of Debye temperature, Θ_D of Mo_2Ga_2C at $P = 0$ GPa. The inset of the figure shows Θ_D as a function of pressure at room temperature. The Debye temperature of Mo_2Ga_2C is also lower than that of Mo_2GaC in the ambient condition.[15] At a fixed pressure, Θ_D decreases with increasing temperature and at a fixed temperature it increases with increasing pressure. These results indicate the changes of the vibration frequency of particles with pressure and temperature. Most of the other solids have weaker bonds and far lower Θ_D; consequently, their heat capacities have almost reached the classical Dulong–Petit value of $3R$ at room temperature as can be seen from Fig. 6(a). If it seems that the harder the solid, the higher the Θ_D and the slower the classical C_V of $3R$ reached by the solid will be, this is not a coincidence.

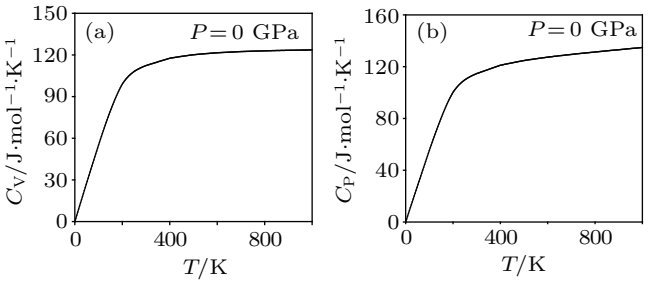


Fig. 6. Temperature dependence of lattice specific heat at constant volume (a) and specific heat at constant pressure (b) of Mo_2Ga_2C.

The lattice heat capacity of a substance is a measure of how well the substance stores heat. The temperature dependence of C_V is governed by the details of vibrations of the atoms and could be determined from experiments. It is worthwhile to outline that the Debye model correctly predicts the low-temperature dependence of the heat capacity at constant volume, which is proportional to T^3.[33] It also recovers the Dulong–Petit law at high temperature.[34] The heat capacities at constant-volume (C_V) and constant-pressure (C_P) of Mo_2Ga_2C each as a function of temperature are displayed in Figs. 6(a) and 6(b). The temperature is limited to 1000 K to reduce the possible effect of anharmonicity. The heat capacities, C_V and C_P both increase with the increase of applied temperature due to the fact that the phonon thermal softening occurs as temperature is increased. The difference between C_P and C_V for the phase is calculated by $\alpha_V^2(T)BTV$, where α_V is the volume thermal expansion coefficient. The difference between heat capacities is very small, which is due to the thermal expansion caused by anharmonicity effects. It is shown in Fig. 6 that the heat capacities of Mo_2Ga_2C increase quickly with increasing temperature in a low temperature range ($T < 300$ K) and thereafter rises slowly up to 700 K and finally approaches to a saturation value. However, in the low temperature region, the heat capacities follow the Debye T^3 power-law whereas at high temperature limit, these approach to the Dulong–Petit limit of $C_V = 3nNk_B = 120$ J/mol·K^{-1}. These results reveal that the interaction between ions in Mo_2Ga_2C has a great effect on heat capacity, especially at low T.

The volume thermal expansion coefficient, α_V, as a function of temperature and pressure is shown in Fig. 7. It is also found that α_V increases rapidly with increasing temperature in a low temperature range of $T < 300$ K and increases gradually after 300 K. The calculated value of α_V at 300 K is

3.6×10^5 K^{-1} which is greater than that of Mo_2GaC[26] due to the lower bulk modulus value of Mo_2Ga_2C than that of Mo_2GaC. It is established that the volume thermal expansion coefficient is inversely related to the bulk modulus of a material. The estimated linear expansion coefficient ($\alpha = \alpha_V/3$) is 1.2×10^{-5} K^{-1}. It can also be found that α_V decreases gradually with increasing pressure.

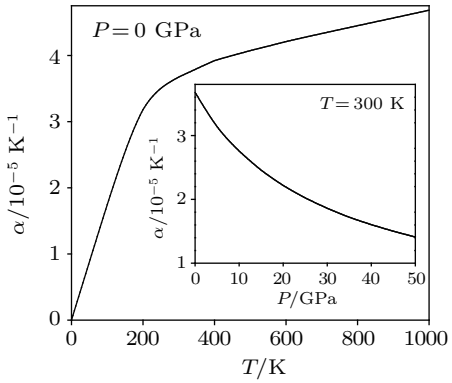


Fig. 7. Plot of volume thermal expansion coefficient versus temperature of Mo_2Ga_2C. The inset shows the pressure dependence.

4. Conclusions

The optical and thermodynamic properties of Mo_2Ga_2C and the prediction of the occurrence of superconductivity are investigated for the first time by the first-principles method. The thermodynamic properties are derived from the quasi-harmonic Debye model with phononic effect. The energy bands around the Fermi level are mainly from Mo 4d states, suggesting that the Mo 4d states dominate the conductivity. The analysis of the electronic band structure indicates the metallic behavior of the compound, which is also confirmed by the studies of absorption and conductivity spectra. All optical functions are calculated in the polarization direction (100) and analyzed in detail. The results are in good agreement with other reported results of Mo_2Ga_2C. The results are also compared with those of the Mo_2GaC, which are available. Based on our present study, it is worthwhile to say that the Mo_2Ga_2C material could be used as a technologically important material.

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