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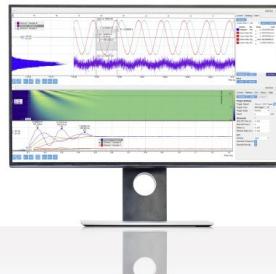
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Mechanical and thermal properties of $\gamma\text{-Mg}_2\text{SiO}_4$ under high temperature and high pressure conditions such as in mantle: A first principles study

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$\gamma\text{-Mg}_2\text{SiO}_4$ is an important mineral in mantle, and our knowledge on its mechanical and thermal properties is critical for many areas of geological sciences. In this work, the crystal structure of $\gamma\text{-Mg}_2\text{SiO}_4$ under high temperature and high pressure conditions is optimized by using the GOMASC method, and the total energy, thermal expansion coefficients, and elastic constants at different temperature and pressure conditions are obtained. On the basis of phonon spectrum, group velocity, phase velocity, Grüneisen parameter, and thermal conductivity are calculated for $\gamma\text{-Mg}_2\text{SiO}_4$ under high temperature and high pressure conditions. These calculated results can provide an important reference for geological research. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4930095>]

I. INTRODUCTION

A basic knowledge of the mechanical and thermodynamic properties of high temperature and high pressure (HTHP) mantle mineral phases is important for understanding the dynamics of earth's mantle.¹ $\gamma\text{-Mg}_2\text{SiO}_4$ (ringwoodite), as a polymorph of olivine, is considered to be the most abundant mineral in the transition zone between 520 and 660 km depth of the earth. Therefore, study of mechanical and thermodynamic properties of $\gamma\text{-Mg}_2\text{SiO}_4$ under HTHP conditions is an important issue in describing and predicting many geological phenomena including earthquake and volcano geological disasters.

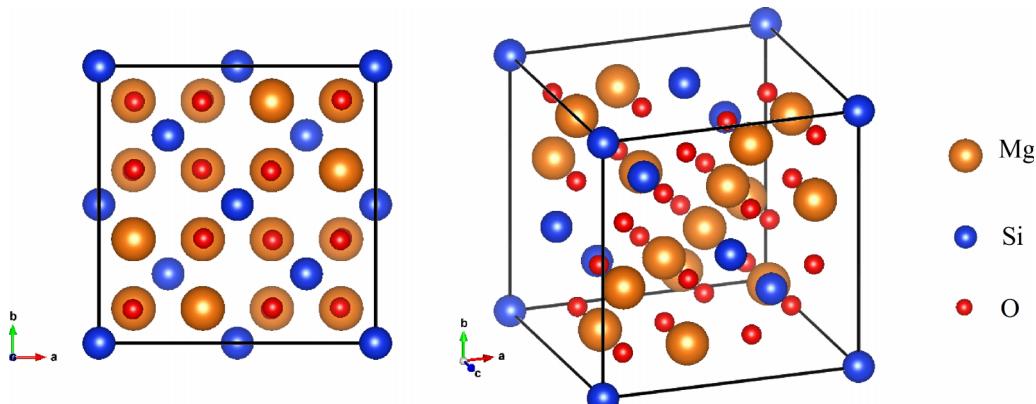
The mechanical and thermodynamic properties of $\gamma\text{-Mg}_2\text{SiO}_4$ were the subjects of a lot of research, both theoretically and experimentally.^{2–6} For example, Price *et al.*^{2,3} studied thermodynamical properties and phase transitions of $\gamma\text{-Mg}_2\text{SiO}_4$ by quasi-harmonic approximation (QHA) method⁷ and its elastic constants at ambient temperature and 5 GPa were calculated. Kiefer *et al.*⁶ calculated the elastic constants, wave velocities of $\gamma\text{-Mg}_2\text{SiO}_4$ as a function of pressure. Masanori and Busing⁴ reported elastic constants of $\gamma\text{-Mg}_2\text{SiO}_4$ under pressure of 5 GPa and ambient temperature conditions. Weidner *et al.*⁵ reported elastic constants of $\gamma\text{-Mg}_2\text{SiO}_4$ determined from Brillouin spectroscopy at ambient conditions. Katsura *et al.*⁸ experimentally measured the thermal expansion coefficients of $\gamma\text{-Mg}_2\text{SiO}_4$ at temperatures from 300 to 2000 K and pressures from 15 to 24 GPa. To the best of our knowledge, the previous computational studies on the mechanical properties of $\gamma\text{-Mg}_2\text{SiO}_4$ have

only been carried out under ambient temperature conditions, but for high temperature elastic properties (e.g., under mantle's temperature and pressure conditions), the results are lacking. At the same time, it is very difficult and expensive to reproduce experimentally the mantle's temperature and pressure conditions and even more difficult to perform precise measurements under these conditions.^{9,10} Recently, a new crystal structure, geometry optimization method for arbitrary symmetry crystals (GOMASC method) has been developed by our group,^{11,12} this makes it possible to calculate HTHP elastic properties for arbitrary symmetry crystals, and it has been applied to MgSiO_3 perovskites and $\alpha/\beta\text{-Nb}_5\text{Si}_3$ phases.^{12,13} In this work, HTHP elastic constants, thermal expansion coefficients, phonon spectrum, phase velocity and group velocity, Grüneisen parameters, and thermal conductivity of the $\gamma\text{-Mg}_2\text{SiO}_4$ have been studied on the basis of the GOMASC method.

II. COMPUTATIONAL DETAILS

In the present work, the calculated lattice structure data are obtained from Ref. 14. As shown in Figure 1, $\gamma\text{-Mg}_2\text{SiO}_4$ belongs to cubic structure with space group of $F\bar{d}3m$, and it contains 56 atoms in its unit cell, in which 32 O atoms occupy the 32e Wyckoff sites, 16 Mg atoms occupy the 16d Wyckoff sites, and 8 Si atoms occupy the 8a Wyckoff sites. The first principles' calculations have been performed by using the Vienna *Ab initio* Simulation Package (VASP)^{15,16} with Projector Augmented Wave (PAW)¹⁷ potential. The exchange-correlation function of the local density approximation (LDA)^{18,19} has been employed. In our calculations, a kinetic cut-off energy of 600 eV is used. The Brillouin zone of the

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FIG. 1. Crystal structure of $\gamma\text{-Mg}_2\text{SiO}_4$.

unit cells has been sampled by a $3 \times 3 \times 3$ k-point mesh. Density of phonon state calculation has been carried out by PHONOPY codes,²⁰ the supercell approach has been employed, and $1 \times 1 \times 1$ supercells have been used.

In this work, the GOMASC method has been used to calculate the HTHP elastic properties and thermal conductivity of cubic $\gamma\text{-Mg}_2\text{SiO}_4$. For cubic crystal structures, the deformed crystal configuration tensor X can be expressed as

$$\begin{aligned} X &= X_0 \cdot [1 + \varepsilon] = X_0 \cdot \left[1 + \begin{pmatrix} e_{xx} & e_{xy}/2 & e_{xz}/2 \\ e_{yx}/2 & e_{yy} & e_{yz}/2 \\ e_{zx}/2 & e_{zy}/2 & e_{zz} \end{pmatrix} \right] \\ &= a_0 \cdot \left[1 + \begin{pmatrix} e_{xx} & e_{xy}/2 & e_{xz}/2 \\ e_{yx}/2 & e_{yy} & e_{yz}/2 \\ e_{zx}/2 & e_{zy}/2 & e_{zz} \end{pmatrix} \right], \end{aligned} \quad (1)$$

where X_0 is the initial crystal configuration tensor, ε is the strain tensor, a_0 is the primitive unit cell lattice constant, and e_{ij} ($i, j = x, y$, and z) are the strain components in Cartesian coordinates.

The non-equilibrium Gibbs free energy at temperature T and pressure P is a function of X given by

$$G[X, T] = E_{\text{stat}}[X(\varepsilon)] + F_{\text{vib}}[X(\varepsilon); T] + PV[X(\varepsilon)], \quad (2)$$

where $E_{\text{stat}}[X(\varepsilon)]$ and $F_{\text{vib}}[X(\varepsilon); T]$ are the total energy at 0 K and 0 GPa, and the lattice vibration Helmholtz free energy, respectively. $F_{\text{vib}}[X(\varepsilon); T]$ can be calculated from phonon frequency as follows:

$$\begin{aligned} F_{\text{vib}} &\left[X(\varepsilon); T \right] \\ &= \int_0^{\infty} \left\{ \frac{1}{2} \hbar \omega + k_B T \ln(1 - e^{-\hbar \omega / k_B T}) g[X(\varepsilon); \omega] \right\} d\omega, \end{aligned} \quad (3)$$

where ω is the phonon frequency, k_B is the Boltzmann constant, \hbar is the reduced Planck constant, and g is phonon density of states.

The equilibrium Gibbs free energy can be calculated by minimizing Eq. (2) with respect to the strain ε as follows:

$$\begin{aligned} G^* &\left[\varepsilon_0^T; T \right] = \min_{\varepsilon} \{E_{\text{stat}}[X(\varepsilon)] \\ &+ F_{\text{vib}}[X(\varepsilon); T] + PV[X(\varepsilon)]\}. \end{aligned} \quad (4)$$

Based on Eq. (4), the equilibrium strain ε_0^T at a fixed temperature T is acquired. As ε_0^T is a function of lattice lengths a, b, c and lattice angles α, β, γ , there is

$$f_{i(i=1,2,3,4,5,6)}(a, b, c, \alpha, \beta, \gamma, (\varepsilon_0^T)_{i(i=1,2,3,4,5,6)}) = 0, \quad (5)$$

where $f_{i(i=1,2,3,4,5,6)}$ represents the multi-variable function of lattice parameters and equilibrium strain ε_0^T . By solving Eq. (5), the lattice parameters as a function of temperature can be calculated. More calculated details can be found in Refs. 11 and 12.

III. RESULTS AND DISCUSSION

A. The optimized lattice parameters and thermal expansion coefficients

Based on the crystallographic data of $\gamma\text{-Mg}_2\text{SiO}_4$,¹⁴ the HTHP lattice parameters and the internal coordinates of atoms are optimized by the GOMASC method^{11,12} under pressures of up to 30 GPa and temperature from 300 to 1800 K. Next, the HTHP thermal expansion coefficients of $\gamma\text{-Mg}_2\text{SiO}_4$ crystal are obtained.²¹ The optimized lattice parameters at ambient conditions are compared with previous theoretical and experimental values, as shown in Table I. Our results by using the LDA functional are slightly lower than the experimental values, but show a good agreement with previous theoretical data.^{14,22,23}

The volume thermal expansion coefficients α_V are defined as²¹

$$\alpha_V = \frac{1}{V_0} \cdot \frac{dV}{dT}, \quad (6)$$

in which V_0 is the equilibrium volume at temperature of 300 K and V is the lattice volume at temperature T .

By using Eq. (6), volume thermal expansion coefficients α_V of $\gamma\text{-Mg}_2\text{SiO}_4$ under HTHP conditions have been calculated and they are shown in Figure 2. As seen in Figure 2, at 300 K, with increasing pressure, the volume of $\gamma\text{-Mg}_2\text{SiO}_4$ decreases. More specifically, the volumes are compressed by 4.4%, 8.2%, and 11.3% at pressures of 10, 20, and 30 GPa, respectively. At a given pressure, the lattice volume increases monotonously with increasing temperature and the volumes are inflated by 4.3%, 3.1%, 2.5%, and 2.2% with temperature increasing from 300 to 1800 K at the pressures of 0, 10,

TABLE I. Space groups, atomic coordinates, and optimized lattice parameters of $\gamma\text{-Mg}_2\text{SiO}_4$; comparison with previous experimental and theoretical values at ambient conditions.^{14,22,23}

Phase	Space groups	Atomic coordinates			a (Å)
$\gamma\text{-Mg}_2\text{SiO}_4$	$Fd\bar{3}m$	Si	8a	(0, 0, 0)	8.01 ^a
		Mg	16d	(0.625, 0.625, 0.625)	7.79, ^b 7.93, ^c 8.065 ^d
		O	32e	(0.372, 0.372, 0.372)	

^aCalculated lattice parameters in present work.

^bTheoretical lattice parameters from Ref. 22.

^cTheoretical lattice parameters from Ref. 14.

^dExperimental lattice parameters from Ref. 23.

20, and 30 GPa, respectively. By comparing with previous experimental values, our calculated thermal expansion coefficient of 1.74×10^{-5} K⁻¹ at 0 GPa and 300 K agrees well with experimental values of 1.9×10^{-5} K⁻¹, 1.76×10^{-5} K⁻¹, and 1.84×10^{-5} K⁻¹ by Piekarz,²⁴ Suzuki,²⁵ and Chopelas,²⁶ respectively. When the temperature is below 1000 K, limited by the accuracy of measurement approach, it is clearly seen that there are some errors among the experimental values, but the calculated thermal expansion coefficients are within the range of them, and the deviation between calculated and experimental values is $\sim 8\%$. At the same time, the magnitude of $\gamma\text{-Mg}_2\text{SiO}_4$'s thermal expansion coefficients is the same as that of Mg₂SiO₃ perovskites.¹² Our results have also indicated that α_V of $\gamma\text{-Mg}_2\text{SiO}_4$ decreases monotonically with pressure, which means that the thermal expansion is suppressed by the pressure. In other words, the effect of pressure on thermal expansion becomes less significant with increasing pressure.

B. Temperature-dependent elastic constants

Elastic constants are important parameters to represent materials' elastic properties.¹³ They also can be used for better understanding crystal's structural stability.²⁷ Based on the GOMASC method, optimized lattice parameters of $\gamma\text{-Mg}_2\text{SiO}_4$ under HTHP conditions have been obtained. Furthermore, the HTHP elastic constants of $\gamma\text{-Mg}_2\text{SiO}_4$

have been calculated by using the deformation method proposed by Zhao.⁷ The details on the computational method for HTHP elastic constants have been described in our earlier publications.^{11,12} In brief, isothermal elastic constants can be considered as strain derivatives of the Helmholtz free energy. According to the continuum elasticity theory^{28,29} and QHA approach,⁷ the Helmholtz free energy under deformed crystal configuration $X(\varepsilon)$ can be described as

$$F[X(\varepsilon), T] = E_{stat}[X(\varepsilon)] + F_{vib}[X(\varepsilon); T], \quad (7)$$

where $E_{stat}[X(\varepsilon)]$ is the 0 K static energy as a function of $X(\varepsilon)$. $F_{vib}[X(\varepsilon); T]$ is the lattice vibration free energy which can be determined by phonon frequency as follows:

$$F_{vib}[X(\varepsilon); T] = \int_0^\infty \left\{ \frac{1}{2} \hbar \omega + k_B T \ln(1 - e^{-\hbar \omega / k_B T}) g[X(\varepsilon); \omega] \right\} d\omega, \quad (8)$$

where ω represents the phonon frequency, k_B is the Boltzmann constant, \hbar is the Planck constant, and g is the phonon density of state.

According to the Taylor series expansion, at a fixed temperature of T , Eq. (8) can be expanded with variable ε as

$$\begin{aligned} F[X(\varepsilon); T] &= F[X(0); T] + \frac{dF[X(\varepsilon); T]}{d\varepsilon} |_{\varepsilon=0} \varepsilon \\ &\quad + \frac{d^2F[X(\varepsilon); T]}{2!d\varepsilon^2} |_{\varepsilon=0} \varepsilon^2 \\ &\quad + \dots + \frac{d^nF[X(\varepsilon); T]}{n!d\varepsilon^n} |_{\varepsilon=0} \varepsilon^n + R_n(\varepsilon). \end{aligned} \quad (9)$$

The temperature and pressure dependent elastic constants could be determined by the second order strain derivatives of the Helmholtz free energy: $\frac{d^2F[X(\varepsilon); T]}{2!d\varepsilon^2}$. Thus, Mg₂SiO₄ decreases elastic constants of cubic structure crystal $\gamma\text{-Mg}_2\text{SiO}_4$, three deformational modes: $[\delta, -\delta, \delta^2/(1 - \delta^2), 0, 0, 0]$, $[\delta^2/(1 - \delta^2), 0, 0, 2\delta, 0, 0]$, and $[\delta, \delta, \delta, 0, 0, 0]$ are used, and their corresponding linear equations are solved to obtain the elastic constants.^{7,11,12} Finally, three independent isothermal elastic constants of c_{11} , c_{12} , and c_{44} for $\gamma\text{-Mg}_2\text{SiO}_4$ have been calculated, as shown in Figure 3. The isentropic elastic constants c_{ij}^S are also computed at 300 K and 0 GPa based on the following equations.¹²

$$c_{ij}^S = c_{ij} + \frac{TV\lambda_i\lambda_j}{C_v}, \quad (10)$$

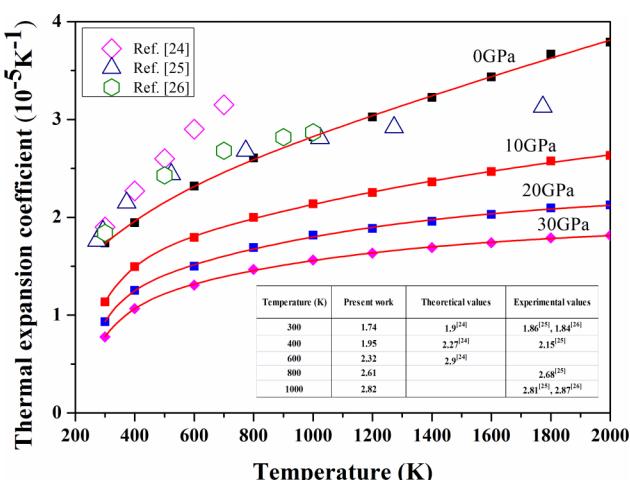


FIG. 2. The HTHP volume expansion coefficients α_T ; comparison with the available theoretical values²⁴ and experimental values.^{25,26}

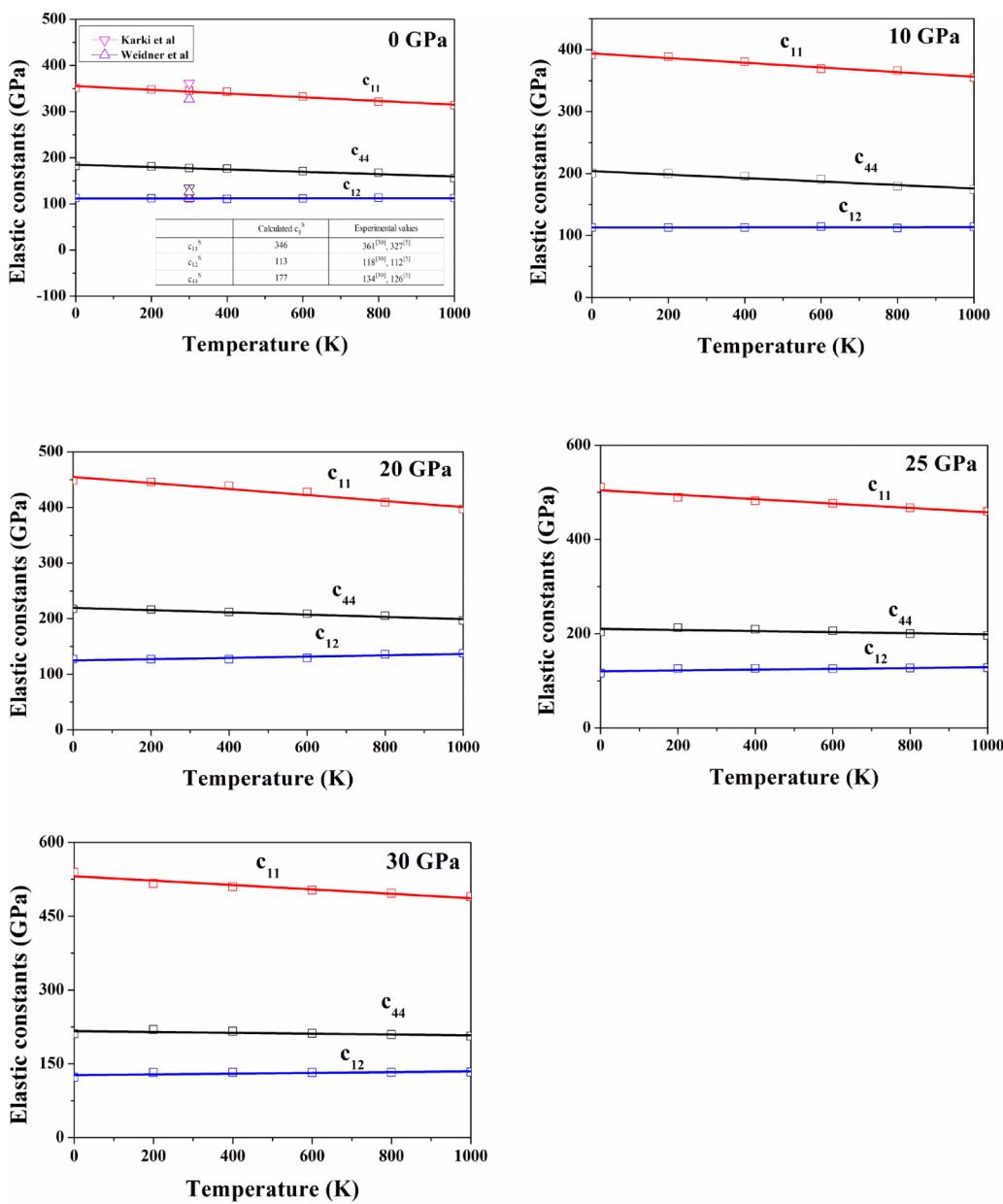


FIG. 3. Temperature dependent isothermal elastic constants of γ -Mg₂SiO₄ at pressures of 0, 10, 20, 25, and 30 GPa.^{5,30}

$$\lambda_i = - \sum_{j=1}^6 \alpha_j c_{ij}, \quad (11)$$

where T, V, and C_v are temperature, volume, and heat capacity, respectively, and α_j is the linear thermal expansion coefficient along the deformed direction j. The calculated isentropic elastic constants are $c_{11}^S = 346$ GPa, $c_{12}^S = 113$ GPa, and $c_{44}^S = 177$ GPa very close to the isothermal values. The calculated elastic constants agree well with available experimental data at 300 K and 0 GPa,^{5,30} further validating our computational method.

Based on the lattice dynamical theory,^{30,31} the three stability criteria for the cubic γ -Mg₂SiO₄ crystal are

$$c_{11} + 2c_{12} > 0, c_{44} > 0, c_{11} - c_{12} > 0, \quad (12)$$

which are connected to the bulk, shear, and tetragonal shear moduli, respectively. They are referred to as spinodal,

shear, and Born criteria, respectively.^{30,31} It is clear from the HTHP elastic constants that γ -Mg₂SiO₄ is in full conformity with the mechanical stability criterion.

As shown in Figure 3, all three independent elastic constants decrease with temperature at pressure of 0 GPa. With temperature increase from 0 to 1000 K, the elastic constants c_{11} , c_{12} , and c_{44} are softened by 19.1%, 20.4%, and 14.3%, respectively. While at pressure of 30 GPa, c_{11} and c_{44} are softened by 9.1% and 2.4%, c_{12} remains almost unchanged. In geological research, HTHP elastic constants present the primary data for modeling geological processes and phenomena.⁶ γ -Mg₂SiO₄ is considered to be the most abundant mineral in the transition zone of earth. Therefore, our calculated results can provide quite important reference data for studying geological processes and phenomena in the transition zone of earth.

C. Phonon spectra and phonon velocities of the $\gamma\text{-Mg}_2\text{SiO}_4$ phase

Phonon spectra are expressed as the relationship between phonon energy and momentum,^{32,33} which plays an important role in the lattice thermal transmission properties.³³ In this work, the phonon dispersion curves along the high-symmetry directions in the Brillouin zone and phonon density of states at 0 GPa and 30 GPa have been calculated by using PHONOPY codes,²⁰ and they are shown in Figure 4. Because the primitive unit cell contains 56 atoms, the complete phonon spectrum consists of 168 dispersion curves in the Brillouin zone, including 3 branches representing the acoustic branch and the rest of the 165 branches representing the optical branch. It can be seen that no imaginary phonon frequency is observed, which indicates that the $\gamma\text{-Mg}_2\text{SiO}_4$ is a dynamically stable phase. At Γ point, there are three acoustic branch waves, including two degenerate transverse waves and a nondegenerate longitudinal wave. For the acoustic wave, when \mathbf{k} point is near Γ point, the frequency is directly proportional to the wave vector. When the \mathbf{k} point is close to the edge of Brillouin zone, the short wavelength is close to the lattice constant, and the continuous elastic medium model is no longer used in this case. To further study the effect of pressure on phonon spectra, the phonon spectra and phonon density of states for $\gamma\text{-Mg}_2\text{SiO}_4$ have been calculated under 30 GPa. They are shown in Figures 4(c) and 4(d), respectively. With

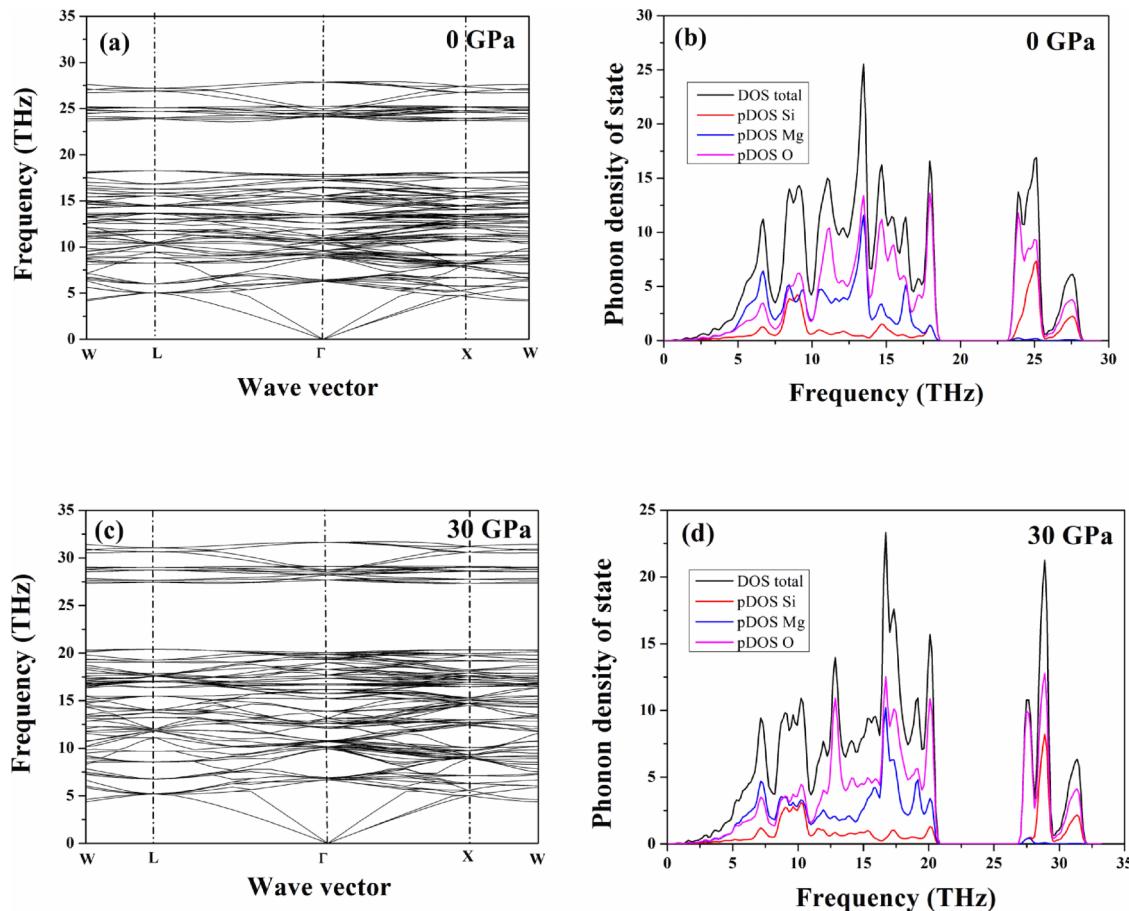


FIG. 4. Phonon dispersion curves along high-symmetry directions in the Brillouin zone and phonon density of states for $\gamma\text{-Mg}_2\text{SiO}_4$. (a) Phonon dispersion curves at 0 GPa, (b) phonon density of states at 0 GPa, (c) phonon dispersion curves at 30 GPa, and (d) phonon density of states at 30 GPa. Note that the high-symmetry points in units are Γ (0,0,0), L (0.5,0.5,0.5), X (0.5,0,0.5), and W (0.5,0.25,0.75), respectively.

increasing pressure, the maximum frequency in spectrum is increasing.

The phonon velocities are relevant to the phonon transportation in crystal. Recall that the group velocity and phase velocity are defined as^{33–36}

$$v_p = \frac{\omega(k)}{k}, \quad (13)$$

$$v_g = \nabla_k \omega(k), \quad (14)$$

where v_p is the phase velocity and v_g is the group velocity, ω is the wave's angular frequency, and k is the distance between two points in Brillouin zone. As usual, the function $\omega(k)$ represents the dispersion relation.

In this work, the phase velocity and group velocity have been calculated on the basis of the obtained phonon spectrum at pressures of 0 GPa and 30 GPa. These velocities for the $\gamma\text{-Mg}_2\text{SiO}_4$ are shown in Figure 5. It can be seen that the phase velocity of optical phonons is one to two orders of magnitude larger than that of acoustic phonons. At pressure of 0 GPa, the group velocity of the optical branches is generally less than 4000 m/s, while the group velocity of the acoustic branches is distributed in the range of 4000–10 000 m/s. At pressure of 30 GPa, the group velocity of the optical branches is generally less than 6000 m/s, while the velocity of acoustic branches is distributed in the range of 6000–11 000 m/s. At pressure of 0 GPa, the average group velocity and average

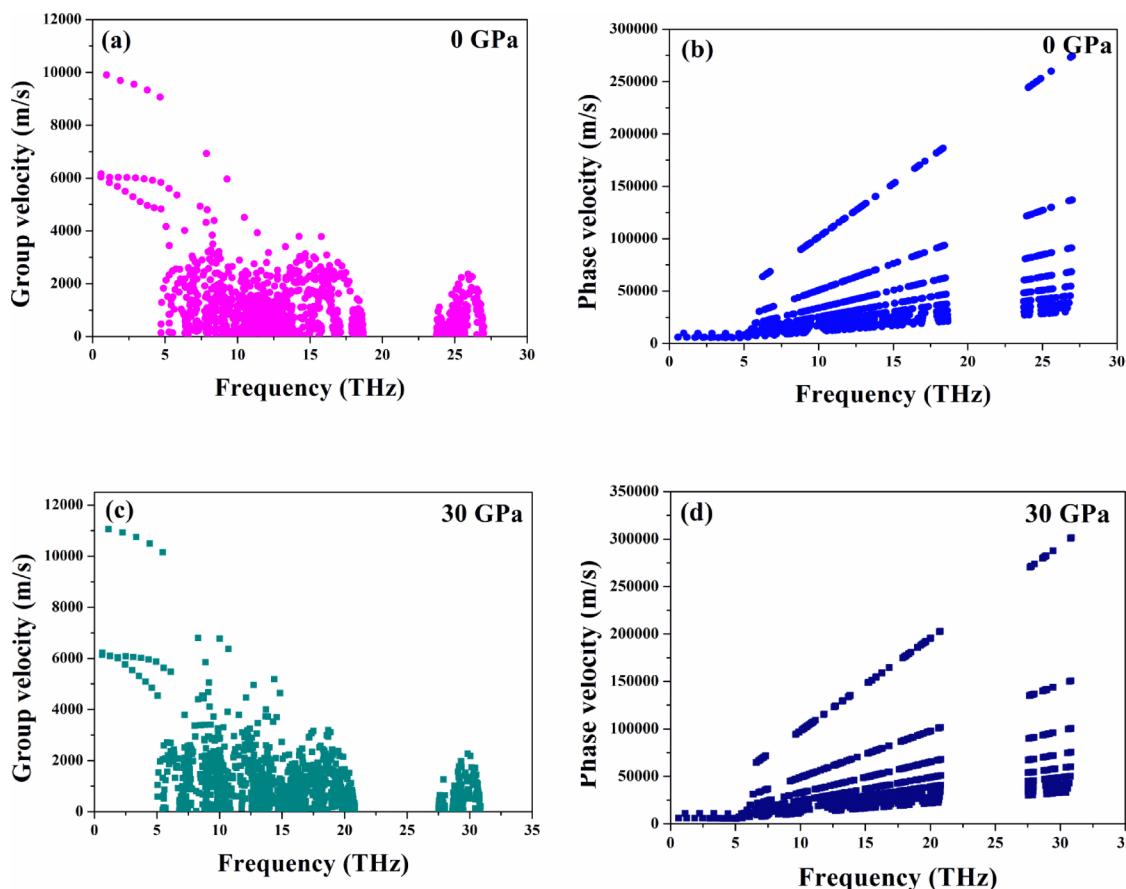


FIG. 5. Phonon group velocity and phase velocity of $\gamma\text{-Mg}_2\text{SiO}_4$ in the [100] direction under different pressure conditions. (a) Phonon group velocity at 0 GPa, (b) phonon phase velocity at 0 GPa, (c) phonon group velocity at 30 GPa, and (d) phonon phase velocity at 30 GPa.

phase velocity are 1011 m/s and 45 968 m/s, respectively, while at pressure of 30 GPa, the average group velocity and average phase velocity are 1076 m/s and 50 989 m/s, respectively. With pressure increasing from 0 GPa to 30 GPa, the average group velocity and average phase velocity are increased by $\sim 6.5\%$ and $\sim 10.9\%$, respectively. It can further be shown that the pressure has a significant effect on the group velocity. Moreover, we can deduce that the seismic wave speed becomes slow when it is transmitted from earth's interior to surface, due to the pressure reduction from earth's interior to surface. Therefore, our calculated pressure dependent group velocity and phase velocity of the $\gamma\text{-Mg}_2\text{SiO}_4$ have significant applications in predicting seismic propagation times.

D. Grüneisen parameters and thermal conductivity

Grüneisen parameters serve as an important characteristic in lattice dynamics. They can quantitatively describe atomic enharmonic vibration effects in crystals.³³ In this work, the Grüneisen parameter of $\gamma\text{-Mg}_2\text{SiO}_4$ is calculated by equation,^{33,37}

$$\gamma = \frac{\alpha \cdot B \cdot V}{C_v}, \quad (15)$$

where the γ is the Grüneisen parameter, α is the volume thermal expansion coefficient, B is the bulk modulus, V is the volume, and C_v is the heat capacity. Thermal conductivity represents the property of heat conduction of materials.³⁸

In the present work, thermal conductivity of $\gamma\text{-Mg}_2\text{SiO}_4$ is calculated by equation,^{33,37}

$$\lambda = A \frac{\overline{M} \cdot \Theta^3 \cdot \delta}{\gamma^2 \cdot N^{2/3} T}, \quad (16)$$

where N is the number of atoms in the primitive unit cell, δ^3 is the volume per atom, \overline{M} is the average mass of the atoms in the crystal, and A is a collection of physical constants ($A \approx 3.1 \times 10^{-6}$ if λ is in W/mK, \overline{M} is in amu, and δ is in Å), the γ is the Grüneisen parameter which can be calculated by the Eq. (15). Finally, Θ in Eq. (16) is the Debye temperature, and it can be calculated by equation,³⁹

$$\Theta = \frac{\omega_D \cdot \hbar}{k_B}, \quad (17)$$

in which ω_D is the maximum frequency from the phonon spectrum, the \hbar is the Planck constant, and the k_B is the Boltzmann constant. As shown in Figure 4, the maximum frequency of the phonon spectrum for $\gamma\text{-Mg}_2\text{SiO}_4$ is 27.9 THz; therefore, the Debye temperature of $\gamma\text{-Mg}_2\text{SiO}_4$ can be deduced as 1340 K.

By using Eqs. (15) and (16), Grüneisen parameters and thermal conductivity of $\gamma\text{-Mg}_2\text{SiO}_4$ have been calculated and the results are displayed in Figure 6. As shown in Figure 6, the values of Grüneisen parameters are distributed in the range from 0.8 to 1.4, and they are increasing with temperature and decreasing with pressure. At a given temperature, Grüneisen parameters are linearly decreasing

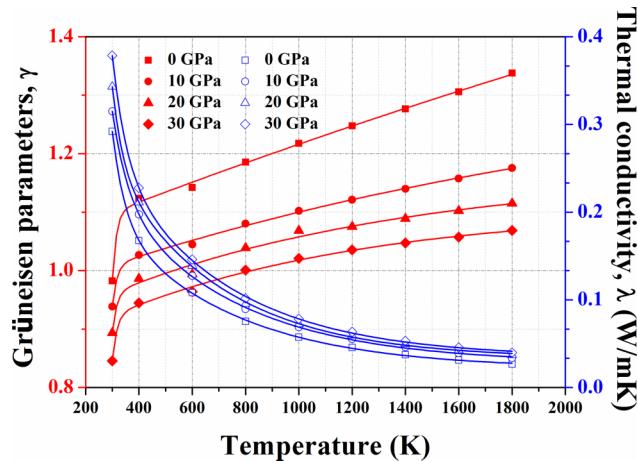


FIG. 6. Grüneisen parameters and thermal conductivity of γ -Mg₂SiO₄ at pressure from 0 to 30 GPa and temperature from 300 to 1800 K.

with pressure. Values of thermal conductivity are distributed in the range of 0–0.4 W/mK. The thermal conductivity decreases dramatically with temperature at lower temperature range, while it decreases gently at temperatures near the melting point. At a given temperature, the thermal conductivity of γ -Mg₂SiO₄ increases with pressure. In geological research, Grüneisen parameter of γ -Mg₂SiO₄ can be applied directly in the study of the mantle phase transition temperature and pressure. When the Grüneisen parameters are calculated, by using them, isentropic and isothermal lines can also be calculated.⁴⁰

IV. CONCLUSIONS

In summary, thermal expansion coefficients, HTHP elastic constants, phonon spectrum, phase velocity and group velocity, Grüneisen parameters, and thermal conductivity under different temperature and pressure conditions have been calculated for γ -Mg₂SiO₄. At ambient conditions, the thermal expansion coefficient calculated in this work is 1.74×10^{-5} K⁻¹. At the temperature of 300 K, elastic constants c₁₁, c₁₂, and c₄₄ calculated in this work are 345 GPa, 112 GPa, and 177 GPa, respectively. At the pressure of 0 GPa, the maximum frequency in the spectrum of γ -Mg₂SiO₄ is 27.9 THz; therefore, the Debye temperature of γ -Mg₂SiO₄ can be deduced as 1340 K. It is found that the average phase velocity and average group velocity of γ -Mg₂SiO₄ at ambient conditions are 45 968 m/s and 1011 m/s, respectively. At ambient conditions, the calculated Grüneisen parameter is 0.98 and thermal conductivity is 0.29 W/mK. The obtained results for elastic and thermodynamic properties are in good agreement with the available experimental and theoretical values. These calculated results can provide an important reference for geological research and contribute to the future experimental and theoretical researches on γ -Mg₂SiO₄.

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