Comparative study on high-pressure physical properties of monoclinic MgCO₃ and Mg₂CO₄

Zi-Jiang Liu¹,², Tian Li³, Xiao-Wei Sun¹, Cai-Rong Zhang⁴ & Jia-Qi Ju¹

The physical properties of Mg-carbonate at high temperature and pressure are crucial for understanding the deep carbon cycle. Here, we use first-principles calculations to study the physical properties of MgCO₃-C2/m and Mg₂CO₄-P2₁/c under high pressure. The research shows that the structure and equation of state of MgCO₃-C2/m are in good agreement with the experimental results, and the phase transition pressure of MgCO₃ from pnma to P2₁/c structure is 44.66 GPa. By comparing the elastic properties, seismic properties, and anisotropy of MgCO₃-C2/m and Mg₂CO₄-P2₁/c, it is found that the elastic modulus and sound velocity of MgCO₃-P2₁/c are smaller than those of MgCO₃-C2/m, while the anisotropy is larger than that of MgCO₃-C2/m. These results indicate that MgCO₃-P2₁/c exists in the deep mantle and may be the main reason why carbonate cannot be detected. The minimum thermal conductivity of MgCO₃-C2/m and Mg₂CO₄-P2₁/c is the largest in the [010] direction and the smallest in the [001] direction. The thermodynamic properties of MgCO₃-C2/m and Mg₂CO₄-P2₁/c are predicted using the quasi-harmonic approximation (QHA) method.

Magnesite (space group R3̅c) is subducted into the deep mantle as the primary carbon carrier, and its high-temperature and high-pressure physical properties are critical for understanding the deep carbon cycle. Previous studies have mainly focused on the structural phase transition of MgCO₃-R3̅c under high-temperature and high-pressure conditions, transforming to monoclinic MgCO₃ (space group C2/m) at around 80 GPa. Oganov et al. used the USPEX method to predict for the first time that MgCO₃-C2/m is most stable in the lower mantle greater than 82.4 GPa. MgCO₃-C2/m has 30 atoms, in which adjacent oxygen atoms form tetrahedra around carbon atoms, and Mg atoms are in octet and tenfold coordination. Subsequently, the structure of MgCO₃-C2/m was verified experimentally and theoretically. Recently, Gavryushkin et al. used USPEX and AIRESS methods to find that MgCO₃ reacts with MgO to form Mg₂CO₄, which has two structures, orthorhombic (space group Pnma) and monoclinic (space group P2₁/c), and its structure is P2₁/c when the pressure is higher than 50 GPa. Their experiments later confirmed the existence of Mg₂CO₄-P2₁/c at the temperature and pressure of the Earth’s lower mantle. Mg₂CO₄-P2₁/c has 28 atoms, it is isostuctural to β-Ca₂SiO₄, and the atoms at the two positions Mg(1) and Mg(2) are six-coordinated, with octahedral coordination polyhedra. Earlier reports, although the structure of Mg₂CO₄ was not determined, believed that it is stable at high pressure.

To understand the carbon cycle in the deep earth, it is crucial to study the structure, phase transition, equations of state, elasticity, thermodynamics, and thermal conductivity of MgCO₃-C2/m and Mg₂CO₄-P2₁/c under high pressure. Recently, Maeda et al. measured the equation of state of MgCO₃-C2/m at high pressure. Since it is extremely difficult to measure the elastic constants, thermodynamic parameters, and thermal conductivity of minerals experimentally, the properties of MgCO₃-C2/m and Mg₂CO₄-P2₁/c have not been reported experimentally. Even the elastic constant of MgCO₃-R3̅c can only be measured to 13.7 GPa, and its thermodynamic properties are only at low pressure, and the results at high pressure are extrapolated.

In the present work, the structures, phase transitions, equations of state, elastic properties, seismic properties, and minimum thermal conductivity of MgCO₃-C2/m and Mg₂CO₄-P2₁/c at high pressure are investigated using first-principles calculations and compared with the available experimental and theoretical results. The QHA method is adopted to research the thermodynamic properties of MgCO₃-C2/m and Mg₂CO₄-P2₁/c.

¹School of Mathematics and Physics, Lanzhou Jiaotong University, Lanzhou 730070, China. ²Department of Applied Physics, Lanzhou University of Technology, Lanzhou 730050, China. ³email: liuzj1024@hotmail.com
Methods

First-principles calculations are used to investigate the high-pressure physical properties of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}/c$ using projector-augmented wave (PAW) as implemented in VASP as implemented in VASP$^{25,26}$. The electronic configurations: 2p$^6$3s$^2$ for Mg, 2s$^2$2p$^2$ for C and 2s$^2$2p$^4$ for O are considered for the valence electrons. The Perdew–Burke–Ernzerhof modified solid (PBEsol) in the generalized gradient approximation (GGA) describes the exchange and correlation potentials. The generation of k-point mesh and the calculation of elastic properties utilize the vaspkit program$^{29}$. The cutoff energy for the plane wave is set to 900 eV. The k-points mesh of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}/c$ are set to 4 × 5 × 5 and 13 × 9 × 7 using the Monkhorst–Pack scheme$^{30}$, respectively. The thermodynamic properties are calculated by the QHA method$^{31}$.

Results and discussion

Structural parameters, phase transition and equation of state. The crystal structures of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}/c$ in the unit cell are shown in Fig. 1. The optimized lattice parameters are summarized in Table 1 and compared with available experimental and previously calculated results. At 110 GPa, the calculated results of MgCO$_3$-C$_2$/m are consistent with the experimental results$^5$. The results for Mg$_2$CO$_4$-P$_{21}/c$ at 100 GPa agree well with the previous calculations$^{14}$. As shown in Fig. 2, the present calculated transition pressure from Mg$_2$CO$_4$-Pnma to Mg$_2$CO$_4$-P$_{21}/c$ is 44.66 GPa, while Gavryushkin et al. calculated 52 GPa$^{14}$. This error may be caused by the use of different exchange correction functions, PBEsol is used in the present work, while PBE was used by Gavryushkin et al.$^{14}$. The accuracy of using PBEsol to calculate the properties of Mg-carbonate has been examined in the previous studies$^{13}$. In the previous study, MgCO$_3$-C$_2$/m was stable in the lower mantle above 80 GPa$^{3,5–13,33}$. Therefore, in order to facilitate comparison, the high-pressure properties of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}/c$ in the pressure range of 50–140 GPa are investigated in this work.

The equations of state for MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}/c$ at 50 to 140 GPa are shown in Fig. 3. It is found that the equation of state of MgCO$_3$-C$_2$/m is in good agreement with available experimental data$^6$. The equation of state of Mg$_2$CO$_4$-P$_{21}/c$ is smaller than that of MgCO$_3$-C$_2$/m, and is almost parallel. The formula unit volume of MgCO$_3$-C$_2$/m is smaller than that of Mg$_2$CO$_4$-P$_{21}/c$, which is in line with their molecular formula composition relationship.

Elastic properties. For monoclinic MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}/c$, there are 13 independent elastic constants (c$_{11}$, c$_{12}$, c$_{13}$, c$_{15}$, c$_{22}$, c$_{23}$, c$_{25}$, c$_{33}$, c$_{35}$, c$_{44}$, c$_{46}$, c$_{55}$ and c$_{66}$). The elastic constants are calculated using the stress–strain method$^{34}$. In this work, all calculated elastic stiffness constants c$_{ij}$ are checked using the mechanical

Table 1. Lattice parameters of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}/c$ at 110 GPa and 100 GPa, respectively, compared with experimental and previous calculations.

| Method                | a (Å) | b (Å) | c (Å) | β  | V(Å$^3$) |
|-----------------------|-------|-------|-------|----|----------|
| MgCO$_3$-C$_2$/m      |       |       |       |    |          |
| This work             | 8.104 | 6.493 | 6.884 | 103.893 | 351.61  |
| Binck et al.$^5$      | 8.117 | 6.510 | 6.911 | 103.858 | 354.64  |
| Mg$_2$CO$_4$-P$_{21}/c$ |     |       |       |    |          |
| This work             | 4.383 | 5.358 | 8.293 | 117.56  | 172.65  |
| Gavryushkin et al.$^{14}$ | 4.408 | 5.383 | 8.345 | 117.65  | 175.39  |

Figure 1. Crystal structures of MgCO$_3$-C$_2$/m (a) and Mg$_2$CO$_4$-P$_{21}/c$ (b) in unit cell. The crystal structures are drawn by VESTA$^{32}$. 

Scientific Reports | (2022) 12:19485 | https://doi.org/10.1038/s41598-022-24033-8
stability criteria and find that they all meet the mechanical stability criteria in the studied pressure range, thus they are mechanically stable.

The elastic constants of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}$/c are plotted in Figs. 4 and 5, respectively. It is found from Fig. 4 that at 50–110 GPa, $c_{22} > c_{33} > c_{11}$, indicating that the a-axis of MgCO$_3$-C$_2$/m is the most easily compressed, and the b-axis is the least compressed. At > 110 GPa, $c_{33} > c_{22} > c_{11}$, the c-axis is least likely to be compressed. From Fig. 5, it can be seen that $c_{22} > c_{11} > c_{33}$ in the studied pressure range, indicating that the c-axis of Mg$_2$CO$_4$-P$_{21}$/c is the most easily compressed, and the b-axis is the least compressible. In the previous study, the elastic constants of MgCO$_3$-R$_3$ are consistent with the experimental results. Therefore, the predicted elastic constants of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}$/c in this work should be correct, but it needs to be further verified by experiments.

Based on the calculated elastic constants, the bulk modulus $B$ and shear modulus $G$ of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}$/c are calculated using the Voigt-Reuss-Hill method. As shown in Fig. 6, the bulk modulus $B$ and shear modulus $G$ of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}$/c increase with increasing pressure, and the bulk modulus $B$ and shear modulus $G$ of MgCO$_3$-C$_2$/m are larger than those of Mg$_2$CO$_4$-P$_{21}$/c at 50–140 GPa.

**Seismic properties.** Based on the calculated bulk and shear moduli and density, the compression ($V_p$) and shear ($V_s$) velocities of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}$/c are given by the following expressions:

**Figure 2.** Enthalpy difference between Mg$_2$CO$_4$-P$_{21}$/c and Mg$_2$CO$_4$-Pnma.

**Figure 3.** Equation of state for MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}$/c.
Figure 4. Elastic constants of MgCO$_3$-C2/m.

Figure 5. Elastic constants of Mg$_2$CO$_4$-P2$_1$/c.
As shown in Fig. 7, the density of Mg\textsubscript{2}CO\textsubscript{4} is larger than that of MgCO\textsubscript{3}, and the difference between their bulk modulus and shear modulus is smaller, respectively. Therefore, the VP and VS of MgCO\textsubscript{3} are larger than those of Mg\textsubscript{2}CO\textsubscript{4} in the studied pressure range, and their VP and VS tend to be parallel, respectively (See Fig. 8).

The VP and VS of MgCO\textsubscript{3} and Mg\textsubscript{2}CO\textsubscript{4} along different directions can be obtained by solving the Christoffel equation\cite{39}:

\[ C_{ijkl}n_i n_j - \rho V^2 \delta_{kl} = 0 \]

In order to visualize the propagation wave velocities of MgCO\textsubscript{3} and Mg\textsubscript{2}CO\textsubscript{4} along different directions, the AWESoMe program\cite{40,41} is used to plot their 3D representations of VP and VS and shear wave splitting and polarization vectors at various pressures (Figs. 9 and 10).

The anisotropy AP of the VP for MgCO\textsubscript{3} and Mg\textsubscript{2}CO\textsubscript{4} is defined as\cite{42}:

\[ A_P = \frac{V_{P,max} - V_{P,min}}{V_{P,aggregate}} \times 100\% \]  

The polarization anisotropy AS of the VS is defined as

\[ V_P = \sqrt{\frac{3B + 4G}{3\rho}} \]  \hspace{1cm} \text{(1)}

\[ V_S = \sqrt{\frac{G}{\rho}} \]  

\[ A_P = \frac{V_{P,max} - V_{P,min}}{V_{P,aggregate}} \times 100\% \]  \hspace{1cm} \text{(2)}

\[ A_S = \frac{V_{S,max} - V_{S,min}}{V_{S,aggregate}} \times 100\% \]  \hspace{1cm} \text{(2)}
The seismic anisotropies of MgCO₃-C₂/m and Mg₂CO₄-P₂₁/c are shown in Fig. 11. The seismic anisotropy of MgCO₃-C₂/m at 75 GPa is found to be in good agreement with the previous theoretical calculations. The anisotropy of Mg₂CO₄-P₂₁/c is obviously larger than that of MgCO₃-C₂/m. The seismic anisotropy of MgCO₃-C₂/m and Mg₂CO₄-P₂₁/c showed obvious nonlinear dependence on pressure. This is mainly due to the nonlinear pressure of wave velocity caused by the nonlinear pressure dependence of the elastic moduli of MgCO₃-C₂/m and Mg₂CO₄-P₂₁/c, especially their shear moduli.

Although the previous experimental and theoretical studies obtained MgCO₃-C₂/m at high temperature and pressure, they did not consider the reaction with MgO, the main mineral of the Earth's lower mantle. The theoretical and experimental results of Gavryushkin et al. show that MgCO₃ reacts with MgO to form Mg₂CO₄-P₂₁/c orthocarbonate under the temperature and pressure conditions of the lower mantle. By comparing the high-pressure physical properties of MgCO₃-C₂/m and Mg₂CO₄-P₂₁/c, it is found that their seismic anisotropy is quite different, while the equation of state, elastic modulus, density and wave velocity have similar relationship with pressure. The low wave velocities of Mg₂CO₄-P₂₁/c are more suitable to explain the existence

\[ A_S = \frac{(V_{S1} - V_{S2})_{\text{max}}}{V_{S_{\text{aggregate}}}} \times 100\% \]  

(4)
of low-velocity zone near the subducting slab. Therefore, we believe that $\text{Mg}_2\text{CO}_4$ may exist in the deep mantle, providing strong evidence for carbon storage in carbonate minerals, which may be the main reason why carbonate rocks cannot be detected in the lower mantle.

**Minimum thermal conductivity.** The thermal conductivity of minerals is critical to understanding the Earth's thermal balance and history. The minimum thermal conductivity of $\text{MgCO}_3$ and $\text{Mg}_2\text{CO}_4$ are calculated using Cahill's model:

$$K_{\text{min}} = \left(\frac{k_B}{2.48}\right)n^{2/3}(v_P + 2v_S)$$

(5)
The anisotropy of the minimum thermal conductivity can be calculated by changing Eq. (5) into the following form:

$$K_{\text{min}} = \left(\frac{k_B}{2.48}\right) n^{2/3} (v_P + v_{S1} + v_{S2})$$

where $k_B$ is Boltzmann’s constant, $n$ is the atomic number density per unit volume. The minimum thermal conductivities of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}$/c are shown in Fig. 12, and it is found that their minimum thermal conductivities increase with the increase of pressure, and that of MgCO$_3$-C$_2$/m is larger than that of Mg$_2$CO$_4$-P$_{21}$/c. In the studied pressure range, $K_{\text{min}}[010] > K_{\text{min}}[100] > K_{\text{min}}[001]$, indicating that the thermal conductivity in the [010] direction is the largest and the thermal conductivity in the [001] direction is the smallest.

**Thermodynamic properties.** Thermodynamic parameters are the preconditions for deriving the thermal state of the Earth’s interior. Therefore, the thermodynamic properties of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}$/c are crucial for studying the thermal state of the lower mantle. The constant volume heat capacity ($C_V$) and the thermal expansion coefficient ($\alpha$) of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}$/c at various pressures are depicted in Figs. 13 and 14, respectively. The $C_V$ and $\alpha$ of MgCO$_3$-C$_2$/m are larger than those of Mg$_2$CO$_4$-P$_{21}$/c under the same pressure.

**Conclusions**

On the basis of verifying the structure and equation of state of MgCO$_3$-C$_2$/m, the phase transition pressure of Mg$_2$CO$_4$-P$_{21}$/c is determined. The high-pressure physical properties of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}$/c at 50–140 GPa are investigated by first-principles calculations. By comparison, it is found that the elastic modulus and wave velocity of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}$/c are smaller than those of MgCO$_3$-C$_2$/m, and the density and seismic anisotropy are larger than those of MgCO$_3$-C$_2$/m. The low wave velocity of Mg$_2$CO$_4$-P$_{21}$/c may be more suitable to explain the existence of the low-velocity zone near the subducting slab. Therefore, it is believed that Mg$_2$CO$_4$-P$_{21}$/c may exist in the deep mantle, providing strong evidence for carbon storage in carbonates and the reason why it cannot be detected in the lower mantle. The minimum thermal conductivity of MgCO$_3$-C$_2$/m is greater than that of Mg$_2$CO$_4$-P$_{21}$/c, and their minimum thermal conductivity is the largest in the [010] direction and the smallest in the [001] direction. The constant volume heat capacity $C_V$ and thermal expansion coefficient $\alpha$ of MgCO$_3$-C$_2$/m are larger than those of Mg$_2$CO$_4$-P$_{21}$/c. Unfortunately, there are no experimental data on the elastic constants, thermodynamic parameters, and minimum thermal conductivity of MgCO$_3$-C$_2$/m and Mg$_2$CO$_4$-P$_{21}$/c, so further verification is required.
Data availability
The datasets used and/or analysed during the current study available from the corresponding author on reasonable request.

Received: 11 October 2022; Accepted: 9 November 2022
Published online: 14 November 2022

References
1. Ishikii, M. et al. Stability of magnesite and its high-pressure form in the lowermost mantle. Nature 427, 60–63 (2004).
2. Plank, T. & Manning, C. E. Subducting carbon. Nature 574, 343–352 (2019).
1. Oganov, A. R., Orso, S., Ma, Y., Glass, C. W. & Garcia, A. Novel high-pressure structures of MgCO3, CaCO3, and CO2 and their role in Earth’s lower mantle. Earth Planet. Sci. Lett. 273, 38–47 (2008).
2. Boulard, E. et al. New host for carbon in the deep Earth. Proc. Natl. Acad. Sci. USA. 108, 5184–5187 (2011).
3. Binck, J. et al. Phase stabilities of MgCO3, and MgCO2-II studied by Raman spectroscopy, X-ray diffraction, and density functional theory calculations. Phys. Rev. Mater. 4, 055001 (2020).
4. Maeda, F. et al. Diamond formation in the deep lower mantle: A high-pressure reaction of MgCO3 and SiO2. Sci. Rep. 7, 40602 (2017).
5. Pickard, C. J. & Needs, R. J. Structures and stability of calcium and magnesium carbonates at mantle pressures. Phys. Rev. B 91, 104101 (2015).
6. Marcondes, M. L., Justo, J. F. & Assali, L. V. Carbonates at high pressures: Possible carriers for deep carbon reservoirs in the Earth’s lower mantle. Phys. Rev. B 94, 104112 (2016).
7. Santos, S. M., Marcondes, M. L., Justo, J. F. & Assali, L. V. C. Stability of calcium and magnesium carbonates at Earth’s lower mantle thermodynamic conditions. Earth Planet. Sci. Lett. 506, 1–7 (2019).
8. Li, Z. & Stackhouse, S. Iron-rich carbonates stabilized by magnetic entropy at lower mantle conditions. Earth Planet. Sci. Lett. 531, 115959 (2020).
9. Tsuchiya, J., Nishida, R. & Tsuchiya, T. First Principles calculation of the stability of Iron bearing carbonates at high pressure conditions. Minerals 10, 54 (2020).
10. Newton, R. C. & Sharp, W. E. Stability of forsterite+CO2 and its bearing on the role of CO2 in the mantle. Proc. Natl. Acad. Sci. USA. 108, 5184–5187 (2011).
11. Tsuchiya, J., Nishida, R. & Tsuchiya, T. First Principles calculation of the stability of Iron bearing carbonates at high pressure conditions. Proc. Japan Acad. Ser. B. 67, 57–60 (1991).
12. Yang, J., Mao, Z., Lin, J. F. & Prakapenka, V. B. Single-crystal elasticity of the deep-mantle magnesite at high pressure and temperature. Earth Planet. Sci. Lett. 392, 292–299 (2014).
13. Litovitz, T. A. Lattice energies, phase transformations and volatiles in the mantle. In: Earth’s Planet. Int. 3, 196–200 (1970).
14. Irving, A. J. & Wyllie, P. J. Melting relationships in CaO-CO2 and MgO-CO2 to 36 kilobars with comments on CO2 in the mantle. Earth Planet. Sci. Lett. 20, 220–225 (1973).
15. Newton, R. C. & Sharp, W. E. Stability of forsterite+CO2 and its bearing on the role of CO2 in the mantle. Earth Planet. Sci. Lett. 26, 239–244 (1975).
16. Katura, T. et al. Stability of magnesite under the lower mantle conditions. Proc. Japan Acad. Ser. B. 67, 57–60 (1991).
17. Kiefer, B., Stixrude, L., Hafner, J. & Kresse, G. Structure and elasticity of wadsleyite at high pressures. Phys. Rev. B 86, 245124 (2012).
18. Selwood, J. et al. Stability of magnesite under the lower mantle conditions. Geochem. Geophys. Geosyst. 12, Q06005 (2011).
19. Muñoz-Santiburcio, D. & Hernández-Laguna, A. AWESoMe 1.1: A code for the calculation of phase and group velocities of acoustic waves. Comput. Phys. Commun. 188, 2232–2248 (2011).
20. Zhang, J., Martinez, I., Guyot, F., Gillet, P. & Saxena, S. K. X-ray diffraction study of magnesite at high-pressure and high-temperature. Phys. Chem. Miner. 24, 122–130 (1997).
21. Kresse, G. & Joubert, D. From ultrasoft pseudopotentials to the projector augmented-wave method. Phys. Rev. B 59, 1758–1775 (1999).
22. Kresse, G. & Furthmüller, J. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. Comput. Mater. Sci. 6, 15–50 (1996).
23. Kresse, G. & Furthmüller, J. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. Phys. Rev. B 54, 11169–11186 (1996).
24. Perdew, J. P. et al. Restoring the density-gradient expansion for exchange in solids and surfaces. Phys. Rev. Lett. 100, 136406 (2008).
25. Wang, Y., Xu, N., Liu, J. C., Tang, G. & Geng, W. T. VASPFT: A user-friendly interface facilitating high-throughput computing and analysis using VASP code. Comput. Phys. Commun. 187, 2003 (2016).
26. Monkhorst, H. J. & Pack, J. D. Special points for Brillouin-zone integrations. Phys. Rev. B 13, 5188–5192 (1976).
27. Otero-de-la-Roza, A., Abbasi-Pérez, D. & Luaña, V. Gibbs2: A new version of the quasiharmonic model code. II. Models for solid-state thermodynamics, features and implementation. Comput. Phys. Commun. 183, 2232–2248 (2012).
28. Monnma, K. & Izami, F. VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data. J. Appl. Crystallogr. 44, 1272–1276 (2011).
29. Zhao, C. S., Lv, C. I., Xu, L. X., Liang, L. & Liu, J. Raman signatures of the distortion and stability of MgCO3 to 75 GPa. Am. Mineral. 106, 367–373 (2021).
30. Wu, T. J. et al. Crystal structures and elastic properties of superhard IrN2 and IrN3 from first principles. Phys. Rev. B 76, 054115 (2007).
31. Hill, R. The elastic behavior of a crystalline aggregate. Proc. Phys. Soc. Lond. 65A, 349–354 (1952).
32. Voigt, W. Lehrbuch der Kristallphysik-mit Ausschluß der Kristalloptik (Vieweg+Teubner Verlag, 1966).
33. Reuss, A. Calculation of yielding mixed crystals plasticity condition for single crystals. Z. Angew. Math. Mech. 9, 49–58 (1929).
34. Anderson, O. L. A simplified method for calculating the debye temperature from elastic constants. J. Phys. Chem. Solids 24, 909–917 (1963).
35. Anderson, D. L. Theory of the Earth (Blackwell Scientific Publications, 1989).
36. Muñoz-Santiburcio, D., Hernández-Laguna, A. & Soto, J. I. AWEsMe: A code for the calculation of phase and group velocities of acoustic waves in homogeneous solids. Comput. Phys. Commun. 192, 272–277 (2015).
37. Muñoz-Santiburcio, D. & Hernández-Laguna, A. AWEsMe 1.1: A code for the calculation of phase and group velocities of acoustic waves in homogeneous solids. Comput. Phys. Commun. 217, 212–214 (2017).
38. Zhou, Y., Dong, Z. Y., Hsieh, W. P., Goncharov, A. F. & Chen, X. J. Thermal conductivity of materials under pressure. Nat. Rev. Mater. 4, 319–335 (2022).

Acknowledgements
This work is supported by the Industrial Support and Guidance Project of Colleges and Universities of Gansu Province (No. 2022CYZC-37), the Key Natural Science Foundation of Gansu Province (No. 20JR5RA211) and the Talent Innovation and Entrepreneurship Project of Lanzhou City (No. 2020-RC-18).
Author contributions
Z.-J.L. designed the calculations and wrote the manuscript. X.-W.S. and C.-R.Z. analyzed the results. J.-Q.J. and T.L. performed partial calculations. All authors reviewed the manuscript.

Competing interests
The authors declare no competing interests.

Additional information
Correspondence and requests for materials should be addressed to Z.-J.L.

Reprints and permissions information is available at www.nature.com/reprints.

Publisher's note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit http://creativecommons.org/licenses/by/4.0/.

© The Author(s) 2022