



Equation of state and structural variations of synthetic forsterite-fayalite solid solution by single-crystal X-ray diffraction

Zhilin Ye¹ · Jingui Xu^{2,3} · Dongzhou Zhang⁴ · Weiyi Liu⁵ · Wenge Zhou³ · Dawei Fan^{2,3}

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Abstract

Olivine, a predominant mineral in the Earth's upper mantle, plays a crucial role in geophysical and geochemical processes due to its abundance and elastic characteristics. This study investigates the elastic properties and structural variations of synthetic forsterite-fayalite solid solutions under high-pressure conditions through synchrotron single-crystal X-ray diffraction. A series of samples with varying fayalite contents were synthesized and characterized to evaluate the impact of Fe incorporation on unit-cell parameters, bulk modulus, and compression behavior. The results demonstrate that increasing fayalite content elongates the *b*-axis, increases polyhedral distortions, and enhances the bulk modulus, while maintaining the structural rigidity of [SiO₄] tetrahedra. By refining the fit parameters of the Birch-Murnaghan equation of state, this study establishes a composition-property relationship for elastic behavior. These results provide key constraints for modeling mantle dynamics and planetary evolution.

Keywords Forsterite-fayalite solid solutions · High pressure · Diamond anvil cell · Elastic property

Introduction

Olivine, as the most predominant rock-forming mineral in the upper mantle, requires precise characterization of its crystal-chemical properties, thermodynamic behavior, and elastic properties to resolve fundamental scientific

questions regarding mantle composition, phase transition mechanisms, and seismic velocity structures (Li and Liebermann 2007; Zhang and Bass 2016; Wei and Shearer 2017; Lapotre et al. 2017; Geiger et al. 2019). Natural olivine is a solid solution of (Mg, Fe)₂SiO₄, ranging between the magnesium-rich end-member forsterite (Fo) and the iron-rich end-member fayalite (Fa). Its composition is commonly expressed using the forsterite number (Fo#) and fayalite number (Fa#), where $Fo\# = 100 \times Mg/(Mg + Fe)$ and $Fa\# = 100 \times Fe/(Mg + Fe)$, with $Fo\# + Fa\# = 100$. Following the recommended notation, the composition is concisely represented as Fo#Fa# (e.g., Fo₉₀Fa₁₀). This composition is primarily controlled by petrogenetic processes and geological environments. For instance, ultramafic rocks (e.g., peridotites, serpentinites) typically host Mg-rich olivine (Fo₈₉Fa₁₁–Fo₉₃Fa₇), reflecting preferential Mg retention during mantle partial melting (Krot et al. 2021). In contrast, basaltic olivines exhibit broader compositional variability (Fo₅₀Fa₅₀–Fo₆₀Fa₄₀), indicative of progressive Fe enrichment during magmatic evolution (Melekhova et al. 2017; Krot et al. 2019). Additionally, serpentinization and mantle metasomatism can change the olivine composition to Fo₈₀Fa₂₀–Fo₈₈Fa₁₈, highlighting Fe migration and redox-driven compositional modification. (Griffioen 2017; Veneranda et al. 2019). These compositional variations

✉ Jingui Xu
xujingui@mail.gyig.ac.cn

✉ Dawei Fan
fandawei@mail.gyig.ac.cn

¹ CNPC Engineering Technology R&D Company Limited, Beijing 102200, China

² State Key Laboratory of Critical Mineral Research and Exploration, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang 550081, China

³ Key Laboratory of High-Temperature and High-Pressure Study of the Earth's Interior, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang 550081, Guizhou, China

⁴ Hawaii Institute of Geophysics and Planetology, School of Ocean and Earth Science and Technology, University of Hawaii at Manoa, Honolulu, HI 96822, USA

⁵ Scripps Institute of Oceanography, La Jolla, San Diego, CA 92093-0244, USA

critically influence olivine's high-pressure compressibility, thereby imposing constraints on the quantitative interpretation of mantle dynamics, including subducting slab recycling and phase transitions in the mantle transition zone.

In the early stages, high-pressure equations of state (EoS) and elastic parameters (e.g., zero-pressure bulk modulus, K_0 , and its pressure derivative, K'_0) for olivine have been systematically investigated using single-crystal/powder X-ray diffraction (XRD). However, discrepancies in experimental methodologies, compositional ranges, and theoretical assumptions have led to persistent controversies over key elastic parameters. Early single-crystal XRD studies revealed considerable variation in the isothermal bulk modulus (K_0) of forsterite, with reported values ranging from 123 to 132 GPa (Zhang 1998; Kroll et al. 2012; Finkelstein et al. 2014). Fayalite showed even wider variability, with K_0 values spanning 113 to 136 GPa (Zhang 1998; Speziale et al. 2004). Such discrepancies likely arose from limited experimental pressure ranges (< 10 GPa) and oversimplified assumptions (e.g., fixed $K'_0 = 4$). A breakthrough occurred when diamond anvil cell (DAC) experiments coupled with single-crystal XRD were employed to systematically investigate the compression behavior of $\text{Fo}_x\text{Fa}_{100-x}$ (Pamato et al. 2019). Their work revealed that the slight increase in olivine bulk modulus with Fe content arises from M2–O and M1–O bond compression disparities that enhance M1O_6 polyhedral rigidity.

Advances in high-pressure single-crystal XRD techniques have reduced parameter inconsistencies, yet systematic discrepancies persist between powder and single-crystal XRD data. A notable example is the 8% variation in K_0 values for Fa_{100} . Andrault et al. (1995) reported 125 GPa from powder XRD data, whereas Zhang (1998) obtained 136 GPa using single-crystal XRD. This discrepancy highlights the methodological sensitivity in determining elastic parameters. The choice of experimental methods can significantly influence the measured values of elastic parameters, implying that their accuracy and reliability are strongly dependent on the specific techniques employed. The K'_0 of forsterite was re-evaluated using high-pressure Brillouin scattering, yielding a value of $4.2(\pm 0.2)$, significantly lower than previous estimates (5.0–5.4) derived from ultrasonic extrapolations (Zha et al. 1996). A refined EoS for $\text{Fo}_{92}\text{Fa}_8$ olivine ($K_0 = 123.4$ GPa, $K'_0 = 5.5$) was later established using high-pressure experiments in the diamond anvil cell and single-crystal XRD studies of natural olivine samples, demonstrating that Mg–Fe substitution within the $\text{Fo}_{92}\text{Fa}_8$ – $\text{Fo}_{62}\text{Fa}_{38}$ range has negligible effects on elastic parameters (Nestola et al. 2011). Their findings also revealed systematic volumetric compression biases introduced by the conventional $K'_0 = 4$ assumption. Subsequent studies integrating single-crystal XRD and molecular dynamics simulations

elucidated olivine's phase transition sequences up to 90 GPa, resolving controversies over metastable phase transitions and amorphization at 35–50 GPa. Nevertheless, the scarcity of single-crystal XRD data at ultrahigh pressures (> 60 GPa) continues to hinder precise elastic modeling of the deep mantle (Finkelstein et al. 2014).

Despite these advances, two interconnected challenges persist. First, existing studies predominantly focus on end-member compositions (Fo or Fa) or limited solid-solution ranges ($\text{Fo}_{92}\text{Fa}_8$ – $\text{Fo}_{80}\text{Fa}_{20}$), leaving a critical knowledge gap in systematic investigations of intermediate Fe-content olivines ($\text{Fo}_{40}\text{Fa}_{60}$ – $\text{Fo}_{80}\text{Fa}_{20}$). This deficiency impedes the development of a universal model linking composition to elastic parameters. Second, methodological disparities (e.g., single-crystal vs. polycrystalline techniques, hydrostatic pressure control) introduce significant scatter in key elastic parameters (e.g., $K_0 = 123$ – 132 GPa and $K'_0 = 4.0$ – 5.5 for forsterite), undermining the reliability of mantle olivine composition inversion and seismic velocity interpretations. Notably, the use of lower-order EoS, such as second-order Birch–Murnaghan (BM2) fits, may systematically underestimate volume changes in subduction zone olivines under mantle transition zone pressures, thereby introducing errors in phase transition depths and slab penetration dynamics (Katsura and Tange 2019). Consequently, developing a high-precision and compositionally comprehensive EoS for olivine is not only critical for high-pressure mineral physics but also essential for resolving mantle chemical heterogeneity, deep volatile cycling, and subduction zone dynamics (Perrillat et al. 2016; Santamaria-Perez et al. 2016; Solomatova et al. 2018).

To address these knowledge gaps, a systematic investigation was conducted on the compositional dependence of elastic parameters and crystal structural evolution across the Fo–Fa solid solution series. High-pressure synchrotron single-crystal XRD experiments were performed on synthetic $\text{Fo}_x\text{Fa}_{100-x}$ olivine samples with a wide compositional range using DAC at ambient temperature. These measurements provide fundamental constraints on compositionally-resolved EoS and crystallographic responses to compression. Furthermore, these results significantly advance our understanding of planetary interior processes by establishing robust structure–property relationships for mantle olivine across key compositional ranges—specifically, forsterite contents (Fo#) between approximately $\text{Fo}_{50}\text{Fa}_{50}$ and $\text{Fo}_{94}\text{Fa}_6$, which are critical for interpreting mechanisms in Earth's upper mantle and other rocky planetary bodies.

Experiments

Sample synthesis

The samples used in this study consist of synthesized solid solutions of forsterite and fayalite end-members (Mg-Fe olivine) with compositions, denoted as Fa_{100} , $\text{Fo}_{10}\text{Fa}_{90}$, $\text{Fo}_{20}\text{Fa}_{80}$, $\text{Fo}_{30}\text{Fa}_{70}$, $\text{Fo}_{40}\text{Fa}_{60}$, $\text{Fo}_{50}\text{Fa}_{50}$, $\text{Fo}_{60}\text{Fa}_{40}$, $\text{Fo}_{70}\text{Fa}_{30}$, $\text{Fo}_{75}\text{Fa}_{25}$, $\text{Fo}_{80}\text{Fa}_{20}$, $\text{Fo}_{95}\text{Fa}_5$, and Fo_{100} . The synthesis experiments were performed using a multi-anvil pressure apparatus (YJ-3000t) at the Institute of Geochemistry, Chinese Academy of Sciences, Guiyang, China.

The starting materials included high-purity magnesium oxide (MgO), ferrous oxide (FeO), and silica (SiO_2) powders, which were mixed in stoichiometric ratios based on the crystal chemical formula. The mixture was then ground for 3 h in acetone using an agate mortar to ensure uniformity. It was then heated in a muffle furnace at 200 °C for over 12 h to eliminate any adsorbed water. Subsequently, the mixtures were placed in platinum capsules containing 1 wt% deionized water. A graphite tube was used as the heater, and pyrophyllite was served as the pressure-transmitting medium. Different compositions of olivine were synthesized under pressures ranging of 1.6–3.4 GPa and temperatures of 950–1050 °C for 48 h.

The synthesized samples exhibited particle sizes of approximately 50–100 μm , with a few particles reaching up to 200 μm . The samples were cleaned with anhydrous ethanol, dried on a heating stage, and well-crystallized grains were selected for further analysis (Fig. 1). Selected grains

were prepared as polished thin sections for both electron microprobe analysis and room-temperature, high-pressure single-crystal XRD experiments, with the XRD samples being double-polished for optimal quality.

Experimental process

Chemical composition analyses were performed using a Shimadzu Corporation EPMA1600 electron probe micro-analyzer at Institute of Geochemistry, Chinese Academy of Sciences, Guiyang, China. Operating conditions were maintained at an accelerating voltage of 25 kV, a beam current of 10 nA, and an electron beam spot size of 5 μm , with counting times of 20 s on peaks and 10 s on backgrounds. The following standards were used: natural quartz (SiO_2) for Si, olivine (Fe_2SiO_4 and Mg_2SiO_4) for Fe and Mg respectively, albite ($\text{NaAlSi}_3\text{O}_8$) and anorthite ($\text{CaAl}_2\text{Si}_2\text{O}_8$) for Na and Ca, while pure metals or simple oxides were adopted for other elements. For each target composition, three single-crystal grains were analyzed to ensure representative sampling (Table 1). The high-pressure synthesis protocol yielded crystalline samples with controlled stoichiometries, as verified through compositional analysis. EMPA measurements revealed minimal deviations (<5%) from nominal Mg concentrations across all synthesized specimens. Additionally, the low standard deviations in Mg molar fraction (0.014–2.58) across multiple sampling points confirmed uniform elemental distribution within individual crystals. These analytical results validate the consistency of both the synthesis methodology and subsequent compositional characterization procedures.

The water content in the synthetic olivine was evaluated using a Nicolet iS50 FTIR spectrometer coupled with a Continuum IR microscope (Thermo Fisher Scientific) at the Institute of Geochemistry, Chinese Academy of Sciences. Characteristic water absorption peaks were observed in the 3700–3000 cm^{-1} range, with water content of 331 ± 99 ppm. Based on previous studies (e.g., Xu et al. 2020), such trace amounts of water have been demonstrated to have no significant effect on the equation of state of olivine.

Room-temperature high-pressure single-crystal XRD experiments were conducted using a symmetric DAC with two configurations: (i) a standard 500 μm culet with a 30° opening angle and (ii) a large-aperture 400 μm culet with a 60° opening angle, designed to maximize angular coverage of diffraction peaks and facilitate structural refinement under high pressure. The sample chamber was created within a rhenium (Re) metal gasket, initially 250 μm thick, which was pre-indented to a final thickness of 50–60 μm . A laser drilling system was used to fabricate a central hole in the gasket, with diameters of approximately 360 μm for the 500 μm culet and 250 μm for the 400 μm culet. Neon

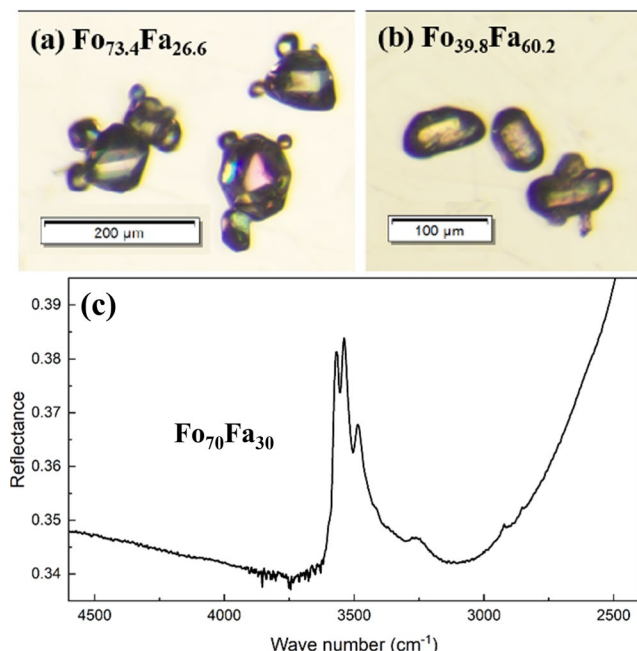
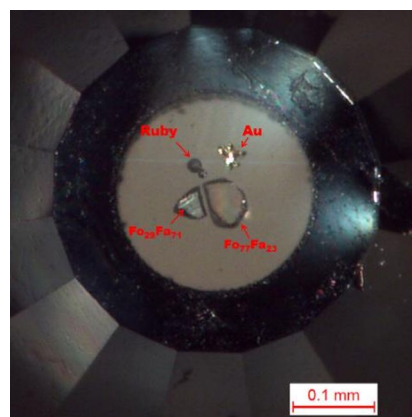


Fig. 1 Representative micrographs of synthesized olivine crystals (a and b) and FTIR spectrum of a representative $\text{Fo}_{70}\text{Fa}_{30}$ crystal (c).

Table 1 Results of electron probe analysis of Mg-Fe olivine solid solutions (wt%)

Nominal compositions	EMPA compositions																		
	Fa ₁₀₀	Fa ₉₀	Fa ₈₀	Fa ₇₀	Fa ₆₀	Fa ₅₀	Fa ₄₀	Fa ₃₀	Fa ₂₀	Fa ₁₀	Fa ₀	Fa ₀	Fa ₀	Fa ₀	Fa ₀	Fa ₀	Fa ₀	Fa ₀	Fa ₀
Standard error of X _{Fa} content (%)	0.021	0.159	0.254	2.14	0.731	0.203	0.137	0.2	0.103	0.225	0.089	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
SiO ₂	29.34(11)	30.46(73)	31.26(9)	32.59(62)	34.17(19)	35.06(20)	36.05(19)	36.85(60)	38.31(10)	39.08(15)	42.95(85)	42.81(2)							
TiO ₂	0.02(1)	0.02(1)	0.01(1)	-	0.02(1)	0.03(1)	0.04(1)	-	0.02(1)	0.02(1)	0.02(1)	0.02(1)							
Al ₂ O ₃	0.01(1)	0.03(1)	0.01(1)	-	0.02(1)	0.03(1)	0.01(1)	0.03(1)	-	0.01(1)	-	0.01(1)							
FeO	70.31(4)	65.26(5)	60.69(10)	54.25(17)	47.66(62)	42.39(8)	35.90(3)	29.31(36)	23.98(2)	20.80(21)	5.52(13)	0.08(1)							
MnO	0.03(1)	0.02(1)	0.02(1)	0.02(1)	0.01(1)	0.01(1)	0.02(1)	-	0.01(1)	-	0.01(1)	-							
MgO	0.01(1)	3.55(2)	7.53(8)	12.41(11)	17.69(94)	21.60(8)	26.20(13)	34.43(33)	37.04(21)	39.85(22)	51.52(1.34)	58.50(26)							
CaO	-	-	-	-	0.01(1)	0.05(1)	0.07(1)	0.01(1)	0.07(1)	-	0.01(1)	0.01(1)							
Na ₂ O	-	0.01(1)	-	0.01(1)	0.03(1)	0.01(1)	-	0.01(1)	0.01(1)	0.01(1)	-	0.01(1)							
Cr ₂ O ₃	0.01(1)	0.01(1)	0.01(1)	0.01(1)	0.01(1)	0.01(1)	0.01(1)	-	0.01(1)	0.01(1)	0.02(1)	0.01(1)							
NiO	-	-	0.01(1)	-	-	0.01(1)	0.01(1)	0.04(1)	0.01(1)	-	0.01(1)	-							
P ₂ O ₅	0.01(1)	0.02(1)	0.01(1)	-	0.02(1)	0.02(1)	0.01(1)	-	0.02(1)	0.01(1)	-	0.02(1)							
Total	99.74(10)	99.37(66)	99.56(4)	99.31(3)	99.64(78)	99.21(31)	98.30(54)	100.67(73)	99.48(53)	99.79(59)	100.05(57)	101.47(39)							

**Fig. 2** Micrograph of sample chamber and water content in Fo₇₇Fa₂₃

gas was loaded as the pressure-transmitting medium via a beamline gas-loading system (Rivers et al. 2008), maintaining the initial chamber pressure below 0.8 GPa. A single-crystal sample ($\sim 40 \times 30 \mu\text{m}^2$) was mounted in the chamber, and pressure was calibrated using the R1 ruby fluorescence band shift and the unit cell volume of Au (Fei et al. 2007). A micrograph of the sample chamber is shown in Fig. 2.

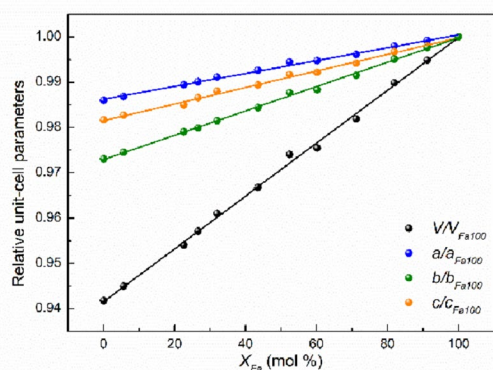
Both ambient-pressure and high-pressure in situ single-crystal XRD experiments were conducted using the same experimental setup at the GeoSoilEnviroCARS (GSE-CARS; Sutton et al. 2022) 13-BMC beamline (Xu et al. 2022) of the Advanced Photon Source (APS), Argonne National Laboratory, USA. The X-ray wavelength was 0.434 Å, and the beam size was $18 \times 12 \mu\text{m}^2$. A Si Pilatus3S 1 M photon counting area detector collected the diffraction signals, while LaB₆ was used as the calibration material (Zhang et al. 2022). During the experiment, the pressure was increased in increments of 1.5–2 GPa using a gas-driven membrane. After stabilizing the pressure for 3 min, single-crystal XRD data were collected with a measurement time of 5 s per step. The pressure inside the sample chamber was measured before and after each data collection using a pressure standard, and the average value was recorded as the actual pressure.

The single-crystal XRD data were processed with Bruker's APEX3 software to determine unit-cell parameters and the crystal's space group from the positions and intensities of the diffraction spots. Structural refinement was based on the *Pbnm* structure model proposed by Smyth and Hazen (Smyth and Hazen 1973) and experimental diffraction intensities. Refinement was performed using OLEX2 and SHELX software (Sheldrick 2008; Dolomanov et al. 2009).

Human Ethics and Consent to Participate declarations: not applicable.

Table 2 Unit-cell parameters and volumes of olivine with various compositions at ambient conditions

Composition $\text{Fo}_{100-x}\text{Fa}_x$	Sigma_X	a (Å)	b (Å)	c (Å)	V (Å ³)	ρ (g/cm ³)
100	0.021	4.8218(1)	10.4803(3)	6.0913(2)	307.817(12)	4.402(1)
91	0.159	4.818(1)	10.4554(2)	6.0792(1)	306.233(8)	4.300(2)
82	0.254	4.812(1)	10.4289(2)	6.0713(1)	304.683(8)	4.196(4)
71	2.14	4.8029(1)	10.3911(2)	6.0558(1)	302.234(8)	4.076(30)
30	0.731	4.7963(1)	10.3577(3)	6.0438(1)	300.245(11)	3.947(10)
52	0.203	4.7951(1)	10.3508(2)	6.0406(1)	299.815(7)	3.839(3)
43	0.137	4.7862(1)	10.3164(3)	6.0264(2)	297.560(10)	3.740(2)
32	0.2	4.7789(2)	10.2856(3)	6.0182(2)	295.817(12)	3.603(3)
27	0.103	4.7740(1)	10.2693(1)	6.0094(1)	294.614(6)	3.540(2)
23	0.225	4.7706(1)	10.2602(2)	5.9996(1)	293.660(12)	3.500(3)
6	0.089	4.7581(2)	10.2126(3)	5.9859(1)	290.869(16)	3.285(1)
0	0.002	4.7540(1)	10.1975(2)	5.9795(1)	289.883(12)	3.208(1)

**Fig. 3** Relative unit-cell parameters of olivines with various compositions at ambient condition

Results and discussion

Synthesis and characterization of Mg-Fe olivine

The compositions of selected Mg-Fe olivine single-crystal grain samples were analyzed using EPMA, and the results are summarized in Table 1. A separate subset of the samples was subjected to single-crystal XRD experiments under ambient temperature and pressure. The diffraction data confirm that the Mg-Fe olivine solid solution crystallizes in the orthorhombic system with the space group *Pbnm*. The corresponding unit-cell parameters and volumes are provided in Table 2.

Figure 3 presents the relationship between the unit-cell parameters of olivine with varying compositions and fayalite end-member content. Note that the error bars are smaller than the symbol sizes and are thus not visible in the plot. The analysis shows that Fe substitution significantly affects the *b*-axis, while the *a*-axis remains minimally influenced. Furthermore, the Mg-Fe olivine binary solid solution

exhibits no excess volume, adhering to the ideal solid solution mixing behavior.

Comparison of unit-cell volumes for olivine of varying compositions under ambient conditions (Fig. 4) reveals a pronounced dependence on composition. As the Fe content increases, the unit-cell volume correspondingly expands. A linear regression of the data points in Fig. 4 establishes the relationship between unit-cell volume (*V*) and the molar fraction of fayalite (X_{Fa}) in the Mg-Fe olivine solid solution series as:

$$V = 289.84(14) + 0.179(3) \times X_{Fa} \quad (1)$$

with an excellent fit indicated by a coefficient of determination (R^2) of 0.998.

Structure refinement of selected Mg-Fe olivine solid solution samples at ambient temperature and pressure was performed, using the olivine structural model proposed by Smyth and Hazen (Smyth and Hazen 1973) as the initial framework. Table 3 shows the average M-O bond length (where M denotes the cation in the X site), the volumes of the [MO₆] octahedra and [SiO₄] tetrahedra, and the distortion indice (*D*) for various compositions along the Mg-Fe solid solution series. The results reveal that Fe incorporation increases the average M1-O and M2-O bond lengths, with a comparable effect on both sites, as Fe is nearly evenly distributed between the M1 and M2 positions. In contrast, the influence on Si-O bond lengths is negligible (Fig. 5a). These findings are consistent with the compression behavior observed across the forsterite-fayalite solid solution, where both end-members exhibit similar polyhedral compression trends. Notably, the M2-O bond remains more compressible than M1-O even with increasing Fe content, supporting the view that the deformation mechanism in olivine is primarily governed by the M2 site. Furthermore, the less compressible nature of the M1 polyhedron with Fe incorporation aligns with the slight increase in bulk modulus toward

Fig. 4 Unit-cell parameters of olivines with various compositions at ambient conditions. The blue data points are referenced from previous studies (Birle et al. 1968; Brown 1973; Hazen 1977; Nover and Will 1981; Kudoh and Takeda 1986; Princivalle and Secco 1985; Aikawa and Tokonami 1987; Bostrom 1987; Motoyama and Matsumoto 1988; Liang and Hawthorne 1994; Yamazaki and Toraya 1999; Kirfel et al. 2005; Nestola et al. 2011)

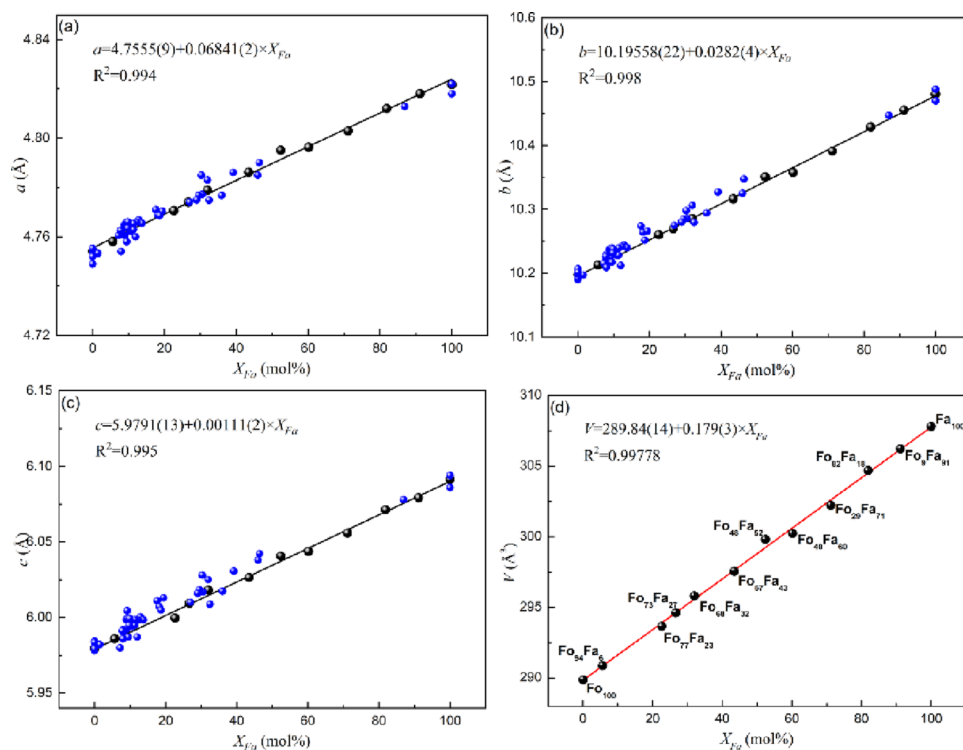
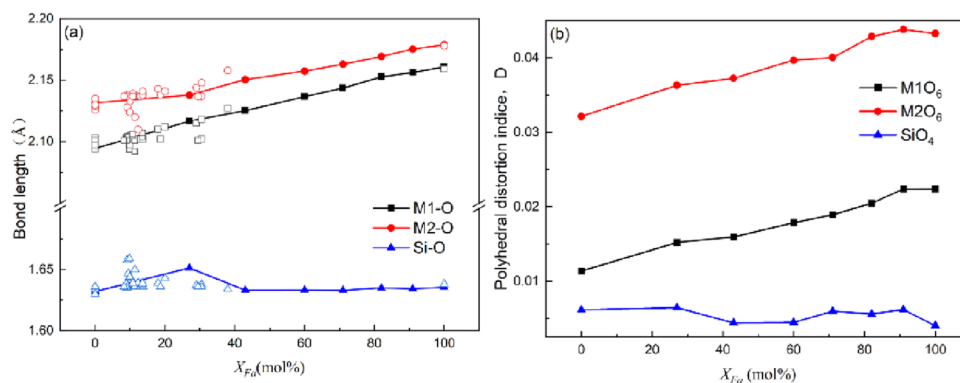


Table 3 Bond length, polyhedral volumes and D values of olivines with various compositions

Composition	Fa ₁₀₀	Fo ₆ Fa ₉₄	Fo ₁₈ Fa ₈₂	Fo ₂₉ Fa ₇₁	Fo ₄₀ Fa ₆₀	Fo ₅₇ Fa ₄₃	Fo ₇₃ Fa ₂₇	Fa ₁₀₀
M1O ₆								
M1-O3(Å)	2.233(3)	2.228(2)	2.219(1)	2.205(3)	2.194(3)	2.176(3)	2.186(3)	2.130(4)
M1-O2(Å)	2.125(3)	2.123(2)	2.120(1)	2.110(2)	2.105(2)	2.096(2)	2.106(2)	2.068(2)
M1-O1(Å)	2.124(3)	2.118(3)	2.119(2)	2.116(2)	2.111(2)	2.1037	2.1193	2.0856
Average bond length(Å)	2.1608	2.1563	2.153(2)	2.1436	2.1366	2.1252	2.1167	2.0945
Polyhedral volume(Å ³)	12.724	12.668	12.627	12.483	12.379	12.208	12.45	11.762
Distortion indices, D	0.0224	0.0224	0.0205	0.0189	0.0179	0.0159	0.0152	0.0114
M2O ₆								
M2-O3(Å)	2.294(3)	2.289(3)	2.282(1)	2.270(2)	2.263(2)	2.249(2)	2.263(2)	2.212(3)
M2-O3(Å)	2.069(3)	2.067(2)	2.065(1)	2.067(2)	2.063(2)	2.066(2)	2.085(2)	2.070(3)
M2-O2(Å)	2.116(3)	2.107(3)	2.099(2)	2.095(3)	2.089(3)	2.081(3)	2.097(3)	2.049(3)
M2-O1(Å)	2.231(3)	2.234(3)	2.222(2)	2.210(3)	2.203(3)	2.194(3)	2.215(3)	2.177(3)
Average bond length(Å)	2.1788	2.1753	2.1692	2.163	2.1574	2.1506	2.1379	2.1316
Polyhedral volume(Å ³)	13.104	13.048	12.963	12.871	12.792	12.698	13.024	12.436
Distortion indices, D	0.0433	0.0438	0.0429	0.04	0.0397	0.0373	0.0363	0.0322
SiO ₄								
Si-O3(Å)	1.634(3)	1.630(2)	1.634(1)	1.631(2)	1.634(2)	1.633(2)	1.650(2)	1.631(2)
Si-O2(Å)	1.649(3)	1.655(3)	1.653(2)	1.652(3)	1.647(4)	1.648(3)	1.673(3)	1.652(3)
Si-O1(Å)	1.625(3)	1.623(3)	1.619(2)	1.618(3)	1.619(4)	1.619(3)	1.632(3)	1.614(3)
Average bond length(Å)	1.6355(4)	1.6344	1.6351	1.633	1.6333	1.6332	1.6514	1.6321
Polyhedral volume(Å ³)	2.2157	2.2116	2.2145	2.2043	2.2051	2.2026	2.2782	2.194
Distortion indices, D	0.004	0.0062	0.0056	0.006	0.0045	0.0044	0.0064	0.0061

Fig. 5 M1-O, M2-O and Si-O bond lengths (a) and polyhedral distortion indices D values (b) of olivine with various compositions at ambient pressure and temperature conditions. The open circle points are referenced from previous studies (Birle et al. 1968; Brown 1973; Hazen 1977; Nover and Will 1981; Bostrom 1987; Motoyama and Matsumoto 1988; Liang and Hawthorne 1994; Kirfel et al. 2005; Pamato et al. 2019)



the fayalite end-member, underscoring a coherent compression motif throughout the solid solution series (Pamato et al. 2019).

The distortion indices, which quantifies the degree of polyhedral distortion, is defined as the deviation of individual cation-oxygen bond lengths from the average bond length. It is calculated using the formula:

$$D = \frac{1}{n} \sum_{i=1}^n \frac{|l_i - l_{avg}|}{l_{avg}} \quad (2)$$

where l_i is the distance from the central cation to the i coordinating oxygen, and l_{avg} is the average bond length. A larger D value indicates a greater distortion, reflecting a greater deviation of the polyhedron from its corresponding ideal shape. As expected from well-established crystal-chemical principles, the data in Fig. 5b confirm that the [M2O₆] octahedron exhibits a significantly larger D value compared to the [M1O₆] octahedron and the [SiO₄] tetrahedron in our samples. The incorporation of Fe has a pronounced impact on the distortion degree of the coordination polyhedra. With increasing Fe content, the distortions of the [M2O₆] and [M1O₆] octahedra become more pronounced, while the distortion of the [SiO₄] tetrahedron remains largely unaffected. These findings highlight the pronounced impact of Fe incorporation on the distortion of coordination polyhedra within the olivine structure.

Equation of state of Mg-Fe olivines

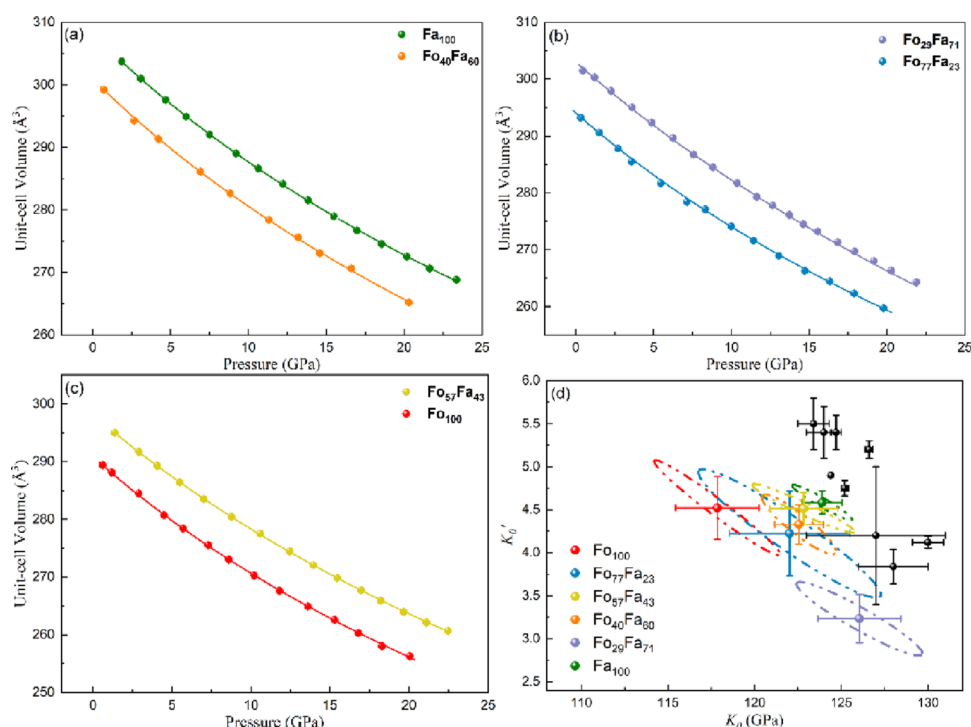
High-pressure single-crystal XRD experiments were performed on six olivine samples with varying compositions: Fa₁₀₀, Fo₂₉Fa₇₁, Fo₄₀Fa₆₀, Fo₅₇Fa₄₃, Fo₇₇Fa₂₃, and Fo₁₀₀. Unit-cell parameters were determined at ambient temperature and high pressure using synchrotron XRD. These results indicate that no phase transitions occurred within the pressure range investigated. All olivine samples retained orthorhombic symmetry within the $Pbnm$ space group.

The pressure-volume (P - V) data were analyzed using the third-order Birch-Murnaghan equation of state (BM3-EoS) (Fig. 6; Table 4). The derived EoS parameters, including the zero-pressure volume (V_0), bulk modulus (K_0), and its first pressure derivative (K'_0) for the Mg-Fe olivine solid solutions are summarized in Table 5. When K'_0 was fixed to 4, the resulting bulk moduli for Fa₁₀₀, Fo₂₉Fa₇₁, Fo₄₀Fa₆₀, Fo₅₇Fa₄₃, Fo₇₇Fa₂₃, and Fo₁₀₀ were 129(1) GPa, 120(1) GPa, 124(1) GPa, 128(1) GPa, 124(1) GPa, and 121(1) GPa, respectively. Notably, no systematic correlation between bulk modulus and composition was observed under this constrained condition. This apparent lack of compositional dependence may be attributed to the strong correlation between K_0 and K'_0 , as evidenced by the confidence ellipse analysis (Fig. 6d). The pronounced negative correlation and narrow, elongated shape of the confidence ellipse indicate that fixing K'_0 at 4 could introduce significant bias in the derived bulk modulus values.

The unconstrained fitting approach yielded physically robust results that better represent the actual material properties. Across the compositional series, most olivine samples exhibited consistent K_0 values ranging from 118(2) to 124(1) GPa, with corresponding K'_0 values between 4.2(5) and 4.58(13). These values show good agreement with literature data for comparable compositions (Andrault et al. 1995; Béjina et al. 2019; Nestola et al. 2011; Kroll et al. 2012; Zha et al. 1998). However, the Fo₂₉Fa₇₁ sample displayed distinct elastic behavior, characterized by an elevated K_0 of 126(2) GPa paired with a reduced K'_0 of 3.3(4). This deviation could originate from either the distinct elastic properties characteristic of this specific composition or artifacts induced by the strong K_0 - K'_0 correlation during fitting of intermediate compositions.

Our analysis further revealed that constraining the zero-pressure unit-cell volume, which was determined from ambient-condition single-crystal diffraction, systematically biased the EoS parameters. The reliability of the derived parameters proved highly sensitive to the accuracy of the zero-pressure volume constraint. When the fixed volume closely matched the true value (e.g., for Fa₁₀₀), the resulting

Fig. 6 Unit cell volume and BM3 EoS fitting line of Mg-Fe olivine solid solutions at different pressure conditions (a–c) and confidence ellipses of K_0 – K'_0 (d). Error bars may be smaller than symbol size (a–c), while the solid black dots represent results from previous studies d (Zhang 1998; Nestola et al. 2011; Kroll et al. 2012; Finkelstein et al. 2014; Pamato et al. 2019)



K_0 values remained accurate. However, imperfect volume constraints led to significant parameter distortions, manifesting as the abnormally low K'_0 for $\text{Fo}_{29}\text{Fa}_{71}$ and artificially high K_0 for Fo_{100} . These findings demonstrate that fixing some of the fit parameters can introduce systematic errors that obscure genuine composition-property relationships. Consequently, all subsequent discussion of compositional effects on the equation of state parameters in Mg-Fe olivine solid solutions relies exclusively on the fully unconstrained fitting results. This approach minimizes artificial correlations between parameters and provides the most reliable representation of the intrinsic material properties across the solid solution series.

Based on our results, the composition dependence of the bulk modulus in Mg-Fe olivine solid solutions is presented in Fig. 7. The data were best described by a second-order polynomial function: $K_0 = 118(1) + 17.18(3)X_{\text{Fa}} - 11.18(2)X_{\text{Fa}}^2$, where X_{Fa} denotes the molar fraction of fayalite component, K' was left free and not fixed to any predetermined value. This equation reveals a positive correlation between bulk modulus and iron content across the olivine solid solution series, indicating that the incorporation of Fe leads to an overall stiffening of the crystal structure.

The EoS parameters for Mg-Fe olivine solid solutions under high pressure exhibit considerable variation across previous studies. For Mg-endmember olivine, reported isothermal bulk moduli (K_0) range from 123 to 136 GPa, while Fe-endmember values span 113–136 GPa, reflecting substantial methodological and compositional uncertainties. A notable limitation in many earlier studies is the assumption

of a fixed K'_0 value of 4, which may introduce systematic bias in K_0 determinations. Strong correlations ($>95\%$) between K_0 and K'_0 during P - V data fitting suggest that constrained K'_0 values could mask genuine compositional effects (Angel et al. 2018).

Experimental determinations of these parameters show significant scatter. Powder XRD measurements yield $K_0 = 130$ GPa with large uncertainties (Andrault et al. 1995), while multi-anvil press in situ XRD studies on Fe-rich compositions report bulk moduli of 128.9–133.4 GPa under an assumed $K'_0 = 5.3$ (Béjina et al. 2019). In contrast, single-crystal XRD analyses of Mg-rich olivine give lower K_0 values (123.4–126.5 GPa) with higher K'_0 estimates (5.1–5.5; (Nestola et al. 2011), the latter being notably higher than the 4.2–4.58 range obtained in the current study. These discrepancies highlight the sensitivity of EoS parameters to experimental techniques and analytical assumptions. Based on previous studies and the results of this work, the relationship between the elastic bulk modulus (K_0) of Mg-Fe olivine solid solutions and the molar iron content (X_{Fa}) can be expressed by the following quadratic equation: $X_0 = 124(2) + 0.030(8)X_{\text{Fa}} - 0.0004(2)X_{\text{Fa}}^2$ ($R^2 = 0.512$), where the numbers in parentheses represent the uncertainties in the last digit of the corresponding coefficients. The discrepancies between the K_0 values obtained in this study and those reported in previous investigations likely originate from differences in experimental and analytical approaches. (1) The use of multi-anvil apparatus in certain previous studies (e.g., Béjina et al. 2019), which involves larger sample volumes but potentially different pressure

Table 4 Unit-cell parameters and volumes of olivine solution at ambient *P-T* conditions

<i>P</i> (GPa)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	<i>V</i> (Å ³)	<i>P</i> (GPa)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	<i>V</i> (Å ³)
Fa ₁₀₀					Fo ₄₀ Fa ₆₀				
1.87(1)	4.8082(2)	10.419(1)	6.063(1)	303.73(4)	0.72(1)	4.791(1)	10.3455(4)	6.0365(2)	299.22(5)
3.10(1)	4.7986(2)	10.370(1)	6.048(1)	300.97(5)	2.67(1)	4.769(1)	10.2697(4)	6.0086(3)	294.28(6)
4.68(1)	4.7873(2)	10.311(1)	6.029(1)	297.60(5)	4.22(6)	4.764(1)	10.2154(7)	5.9866(5)	291.34(8)
6.00(1)	4.7782(2)	10.262(1)	6.014(1)	294.90(5)	6.91(1)	4.740(1)	10.1380(4)	5.9549(3)	286.13(5)
7.51(3)	4.7690(2)	10.208(1)	5.999(1)	292.03(4)	8.83(7)	4.723(1)	10.0876(4)	5.9322(3)	282.62(5)
9.21(2)	4.7582(2)	10.151(1)	5.983(1)	289.00(4)	11.31(4)	4.700(2)	10.0278(6)	5.9067(4)	278.40(10)
10.64(3)	4.7508(3)	10.106(1)	5.970(2)	286.62(6)	13.22(5)	4.685(4)	9.9830(14)	5.8864(10)	275.62(19)
12.21(2)	4.7421(2)	10.059(1)	5.957(1)	284.15(5)	14.62(6)	4.679(3)	9.9424(15)	5.8690(10)	273.05(18)
13.84(5)	4.7341(3)	10.010(1)	5.941(1)	281.54(5)	16.63(8)	4.670(4)	9.9036(15)	5.8516(10)	270.63(19)
15.49(7)	4.7284(3)	9.959(1)	5.925(1)	278.98(5)	20.31(1)	4.641(4)	9.8217(17)	5.8176(12)	265.2(2)
16.97(16)	4.7236(3)	9.911(1)	5.911(2)	276.72(6)					
18.56(9)	4.7189(3)	9.858(2)	5.902(2)	274.53(6)					
20.17(5)	4.7151(4)	9.811(2)	5.891(2)	272.52(7)					
21.65(6)	4.7102(4)	9.768(2)	5.882(2)	270.60(7)					
23.36(11)	4.7073(6)	9.722(2)	5.874(3)	268.81(8)					
Fo ₂₉ Fa ₇₁					Fo ₅₇ Fa ₄₃				
0.45(4)	4.8014(2)	10.371(3)	6.054(1)	301.45(9)	1.38(1)	4.7773(3)	6.012(3)	10.272(1)	295.01(2)
1.18(1)	4.7964(3)	10.358(4)	6.044(1)	300.28(10)	2.91(6)	4.7650(3)	5.990(3)	10.221(1)	291.72(2)
2.22(6)	4.7879(2)	10.317(3)	6.031(1)	297.91(6)	4.08(3)	4.7565(3)	5.975(3)	10.179(1)	289.28(3)
3.55(4)	4.7782(2)	10.266(2)	6.015(1)	295.04(6)	5.49(3)	4.7462(3)	5.9556(3)	10.133(1)	286.42(3)
4.87(2)	4.7707(2)	10.213(3)	6.004(3)	292.36(7)	7.00(1)	4.7359(3)	5.9358(3)	10.085(1)	283.51(3)
6.15(4)	4.7618(3)	10.164(3)	5.984(2)	289.63(8)	8.78(3)	4.7245(3)	5.9148(3)	10.037(1)	280.47(3)
7.44(4)	4.7545(3)	10.105(4)	5.969(4)	286.77(11)	10.58(2)	4.7129(3)	5.8948(3)	9.989(1)	277.51(2)
8.70(1)	4.7475(4)	10.063(5)	5.955(5)	284.51(12)	12.46(4)	4.7013(3)	5.8736(3)	9.938(1)	274.43(2)
10.25(4)	4.7380(7)	10.015(8)	5.938(10)	281.73(14)	13.95(2)	4.6928(3)	5.8575(3)	9.897(1)	272.06(3)
11.44(11)	4.7312(5)	9.963(6)	5.925(7)	279.28(16)	15.47(8)	4.6843(3)	5.8429(3)	9.860(1)	269.86(3)
12.45(11)	4.7248(5)	9.938(7)	5.915(6)	277.75(16)	16.96(6)	4.6778(3)	5.8289(3)	9.819(1)	267.74(3)
13.54(4)	4.7181(5)	9.910(7)	5.904(10)	276.10(17)	18.21(5)	4.6725(3)	5.8163(4)	9.784(1)	265.91(3)
14.46(17)	4.7124(5)	9.881(7)	5.895(7)	274.49(19)	19.65(5)	4.6659(4)	5.8023(4)	9.750(1)	263.95(3)
15.41(21)	4.7065(6)	9.861(8)	5.887(7)	273.20(19)	21.1(1)	4.6591(4)	5.7893(4)	9.719(1)	262.14(3)
16.63(12)	4.6993(5)	9.829(9)	5.874(8)	271.3(2)	22.46(1)	4.6523(4)	5.7794(4)	9.695(1)	260.67(3)
17.73(19)	4.6902(6)	9.808(9)	5.863(10)	269.7(2)					
18.95(25)	4.6869(5)	9.772(8)	5.851(9)	268.0(2)					
20.08(23)	4.6820(6)	9.735(9)	5.843(9)	266.3(2)					
21.69(22)	4.6745(6)	9.701(11)	5.829(10)	264.3(3)					
Fo ₇₇ Fa ₂₃					Fo ₁₀₀				
0.33(1)	4.762(1)	6.007(1)	10.250(1)	293.22(7)	0.61(1)	4.7508(2)	10.194(1)	5.9755(2)	289.40(2)
1.52(3)	4.752(1)	5.993(1)	10.204(1)	290.60(3)	1.22(1)	4.7403(2)	10.190(4)	5.9647(1)	288.12(2)
2.72(8)	4.738(1)	5.983(1)	10.152(1)	287.79(3)	2.93(2)	4.7280(2)	10.139(3)	5.9346(1)	284.47(2)
3.59(5)	4.725(1)	5.976(1)	10.111(1)	285.48(4)	4.54(1)	4.7147(1)	10.071(4)	5.9124(2)	280.73(1)
5.46(5)	4.717(1)	5.947(1)	10.043(1)	281.70(4)	5.75(2)	4.7113(3)	10.024(1)	5.8956(2)	278.41(2)
7.14(6)	4.695(2)	5.933(2)	9.995(1)	278.42(6)	7.33(2)	4.7011(3)	9.979(1)	5.8737(2)	275.55(2)
8.32(3)	4.706(1)	5.914(1)	9.955(1)	277.07(4)	8.66(2)	4.6911(3)	9.942(1)	5.8544(2)	273.05(2)
9.99(3)	4.695(1)	5.895(2)	9.903(1)	274.09(5)	10.25(2)	4.6800(3)	9.899(1)	5.8337(2)	270.27(2)
11.43(5)	4.687(2)	5.879(2)	9.858(1)	271.58(6)	11.84(2)	4.6695(4)	9.859(1)	5.8137(2)	267.63(3)
13.05(3)	4.673(2)	5.867(2)	9.810(1)	268.94(7)	13.62(2)	4.6588(5)	9.816(1)	5.7931(3)	264.92(3)
14.72(5)	4.660(2)	5.851(2)	9.768(1)	266.28(8)	15.33(2)	4.6497(5)	9.779(2)	5.7753(3)	262.59(3)
16.33(4)	4.649(2)	5.837(2)	9.745(1)	264.41(9)	16.81(2)	4.6412(6)	9.742(2)	5.7567(4)	260.30(4)
17.89(4)	4.640(3)	5.820(3)	9.714(2)	262.27(13)	18.32(2)	4.6322(8)	9.708(3)	5.7372(4)	258.02(5)
19.77(4)	4.627(2)	5.808(3)	9.666(2)	259.71(9)	20.15(2)	4.6245(7)	9.682(2)	5.7238(4)	256.29(5)

Table 5 Elastic parameters of Mg-Fe olivine solid solutions

Composition	$V_0(\text{\AA}^3)$	K_0 (GPa)	K'_0	Composition	$V_0(\text{\AA}^3)$	K_0 (GPa)	K'_0
Fa ₁₀₀	308.18(7)	124(1)	4.58(13)	Fo ₅₇ Fa ₄₃	298.31(13)	123(2)	4.51(17)
	307.93(6)	129(1)	4(fixed)		298.02(11)	128(1)	4(fixed)
	307.82(fixed)	129(1)	4.05(14)		297.56(fixed)	132(2)	3.81(20)
Fo ₂₉ Fa ₇₁	303.19 (21)	126 (2)	3.3 (4)	Fo ₇₇ Fa ₂₃	294.05 (8)	122(3)	4.2 (5)
	303.25(12)	120(1)	4(fixed)		294.03(6)	124(1)	4(fixed)
	302.23(fixed)	138(2)	2.19(32)		293.66(fixed)	135(4)	2.76(51)
Fo ₄₀ Fa ₆₀	300.93(13)	123(1)	4.33(23)	Fo ₁₀₀	290.87(4)	118(2)	4.5(4)
	300.72(15)	124(1)	4(fixed)		290.84(2)	121(1)	4(fixed)
	300.25(fixed)	133(4)	3.25(73)		289.88(fixed)	133(4)	2.59(52)

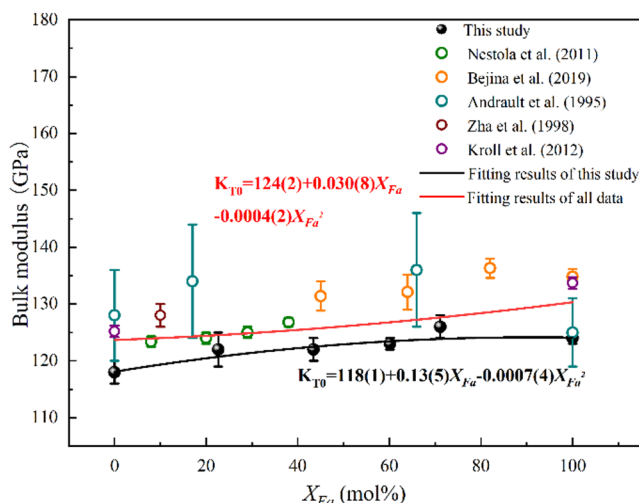


Fig. 7 Correlation between Mg-Fe olivine solid solutions and bulk moduli. The bulk moduli in this study obtained with a freely refined K'_0 . Nestola et al. (2011) used 5.6 for Fo₉₂Fa₈, 5.4 for Fo₈₀Fa₂₀, 5.1 for Fo₇₁Fa₂₉, 5.2 for Fo₆₂Fa₃₈. Andrault et al. (1995) used a fixed K'_0 value of 4 for Fo₁₀₀, Fo₇₃Fa₁₇, Fo₃₄Fa₆₆, Fa₁₀₀ and Béjina et al. (2019) used the same fixed value for Fo₅₅Fa₄₅, Fo₃₆Fa₆₄, Fo₁₈Fa₈₂, Fa₁₀₀. Zha et al. (1998) used 4.2 for Fo₉₀Fa₁₀. Kroll et al. (2012) used 4.1 and 4.75 for Fo₁₀₀ and Fa₁₀₀

environments and stress states compared to DAC experiments; (2) The application of energy-dispersive diffraction techniques (e.g., Andrault et al. 1995), which differ in resolution and data treatment from the angle-dispersive methods employed in our work; (3) Constraints imposed by more limited pressure ranges in some earlier investigations (e.g., Béjina et al. 2019; Nestola et al. 2011), which can affect the robustness of the equation-of-state fitting; (4) The adoption of a BM2 EoS or a BM3 EoS with fixed K' (e.g., Béjina et al. 2019), which assumes a fixed pressure derivative and may not capture the full compression behavior. These differences in experimental setup, pressure range, and data analysis approach are likely responsible for the variations in both the derived moduli and their associated uncertainties. It is noteworthy that Nestola et al. (2011), who used single-crystal XRD in a DAC and a BM3 EoS reported K_0 values for Fo₉₂Fa₈ to Fo₆₂Fa₃₈ olivines that fall within the uncertainty range of our result for Fo₈₀Fa₂₀. This agreement

under comparable experimental conditions reinforces the reliability of the present findings.

Compression and distortion of cation polyhedra

High-pressure single-crystal XRD experiments were conducted on olivine samples with compositions Fo₂₉Fa₇₁ and Fo₇₇Fa₂₃ using a DAC with a wide opening angle. This configuration enabled the collection of a significantly larger number of single-crystal diffraction spots compared to conventional DAC geometries, thereby enhancing the precision of structural refinements. The improved data quality allowed for detailed analysis of bond lengths, polyhedral volumes, and distortion indices for different cation polyhedral (Table 6). These experiments were designed to systematically evaluate the effects of Mg²⁺ and Fe²⁺ substitution on the compressional behavior of olivine, particularly focusing on how iron content influences bond-length variations and polyhedral distortions at high pressures. By comparing the two compositional endmembers, we aim to elucidate the role of cation size and electronic structure in governing phase stability and elastic anisotropy in the olivine system.

According to Anderson and Anderson (1970), the product of bulk modulus and mineral volume remains constant in ionic crystals governed by the Born exponential repulsive potential. However, the experimental results in this study reveal a negative correlation between bulk modulus and mineral volume in Mg-Fe olivine.

In the olivine structure, oxygen atoms form a close-packed arrangement, with two octahedral cation sites (M1 and M2 octahedra) and one tetrahedral cation site (Si tetrahedron). The bulk modulus of a cation coordination polyhedron in silicates is related to its average bond length (d) and cation charge (Z_c), as described by Hazen and Finger (1979):

$$K_P d^3 / Z_c = 7.5 \pm 0.2 \quad (3)$$

where K_P is the bulk modulus of the polyhedron. The bulk modulus of mantle minerals can be approximated as the weighted sum of the bulk moduli of their constituent

Table 6 Average bond length (Å), polyhedral volume (Å³) and distortion indices *D* of Fo₂₉Fa₇₁ and Fo₇₇Fa₂₃ olivine at various pressures

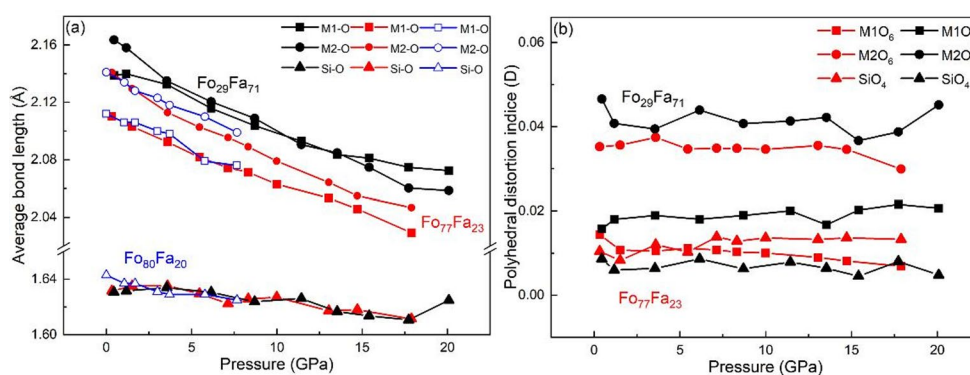
(1) Fo₂₉Fa₇₁										
Pressure(GPa)	0.45(4)	1.18(1)	3.55(4)	6.15(4)	8.70(1)	11.44(1)	13.54(4)	15.41(9)	17.73(9)	20.08(2)
M1O ₆ octahedron										
M1-O3	2.130(13)	2.198(8)	2.193(6)	2.173(7)	2.164(7)	2.156(10)	2.136(10)	2.144(10)	2.137(14)	2.122(13)
M1-O2	2.157(9)	2.111(5)	2.102(4)	2.096(5)	2.082(4)	2.078(6)	2.077(7)	2.071(7)	2.080(10)	2.087(10)
M1-O1	2.131(7)	2.110(7)	2.103(5)	2.078(7)	2.066(6)	2.045(9)	2.038(9)	2.028(8)	2.008(10)	2.008(10)
Average bond length (Å)	2.139(10)	2.140(6)	2.133(5)	2.116(6)	2.104(6)	2.093(8)	2.084(8)	2.081(8)	2.075(10)	2.072(11)
Polyhedral volume (Å ³)	12.39(1)	12.44(1)	12.34(1)	12.10(1)	11.86(1)	11.72(1)	11.57(1)	11.53(1)	11.45(1)	11.47(1)
Distortion indices (<i>D</i>)	0.01573	0.01803	0.01895	0.01807	0.01896	0.02007	0.01671	0.02025	0.02156	0.02065
M2O ₆ octahedron										
M2-O3	2.310(3)	2.264(7)	2.244(5)	2.235(6)	2.212(6)	2.189(8)	2.187(9)	2.157(8)	2.138(12)	2.157(11)
M2-O3	2.084(5)	2.064(5)	2.042(4)	2.025(5)	2.017(5)	2.000(7)	1.997(8)	1.998(7)	1.991(11)	1.987(10)
M2-O2	2.031(15)	2.082(13)	2.068(9)	2.031(11)	2.035(11)	2.013(15)	1.996(16)	2.000(15)	1.962(13)	1.923(13)
M2-O1	2.152(14)	2.210(13)	2.169(9)	2.170(12)	2.159(12)	2.153(16)	2.144(16)	2.138(15)	2.144(19)	2.140(19)
Average bond length (Å)	2.164(9)	2.158(9)	2.135(6)	2.120(8)	2.109(8)	2.091(9)	2.085(12)	2.075(9)	2.060(12)	2.059(9)
Polyhedral volume (Å ³)	12.84(1)	12.78(1)	12.42(1)	12.18(1)	11.99(1)	11.72(1)	11.62(1)	11.45(1)	11.22(1)	11.18(1)
Distortion indices (<i>D</i>)	0.04656	0.04076	0.03942	0.04394	0.04073	0.0413	0.04218	0.03667	0.03877	0.04514
SiO ₄ tetrahedron										
Si-O3	1.602(7)	1.630(6)	1.635(5)	1.633(6)	1.631(6)	1.634(8)	1.622(9)	1.619(8)	1.603(12)	1.610(11)
Si-O2	1.693(16)	1.651(14)	1.653(10)	1.668(13)	1.629(11)	1.635(17)	1.627(17)	1.618(17)	1.642(13)	1.673(13)
Si-O1	1.628(6)	1.615(6)	1.613(5)	1.611(6)	1.603(5)	1.600(7)	1.596(8)	1.599(7)	1.601(10)	1.606(10)
Average bond length (Å)	1.631(11)	1.632(9)	1.634(7)	1.631(9)	1.624(8)	1.626(11)	1.617(12)	1.614(11)	1.611(12)	1.625(11)
Polyhedral volume (Å ³)	2.187(11)	2.199(9)	2.210(8)	2.187(10)	2.163(8)	2.172(13)	2.134(13)	2.122(13)	2.109(13)	2.166(12)
Distortion indices (<i>D</i>)	0.00864	0.00598	0.00639	0.01864	0.00629	0.00789	0.00642	0.00453	0.00803	0.00481
(2) Fo₇₇Fa₂₃										
Pressure(GPa)	0.33(1)	1.52(3)	3.59(5)	5.46(5)	7.14(6)	8.32(3)	9.99(3)	13.05(3)	14.72(5)	17.89(4)
M1O ₆ octahedron										
M1-O3	2.156(6)	2.137(4)	2.125(5)	2.116(4)	2.108(4)	2.103(4)	2.094(4)	2.081(5)	2.071(5)	2.050(7)
M1-O2	2.073(6)	2.085(5)	2.073(5)	2.059(5)	2.048(5)	2.049(5)	2.041(6)	2.037(6)	2.032(7)	2.010(10)
M1-O1	2.101(6)	2.088(4)	2.079(5)	2.069(4)	2.068(5)	2.062(4)	2.054(5)	2.043(6)	2.034(6)	2.028(9)
Average bond length (Å)	2.110(6)	2.103(5)	2.092(5)	2.082(4)	2.074(4)	2.071(5)	2.063(5)	2.053(6)	2.046(6)	2.029(8)
Polyhedral volume (Å ³)	12.01(1)	11.90(1)	11.76(1)	11.57(1)	11.46(1)	11.42(1)	11.31(1)	11.16(1)	11.04(1)	10.78(1)
Distortion indices (<i>D</i>)	0.01442	0.0107	0.01051	0.01114	0.01074	0.01027	0.01005	0.009	0.00814	0.00688
M2O ₆ octahedron										
M2-O3	2.229(6)	2.222(5)	2.213(6)	2.198(5)	2.193(5)	2.185(5)	2.173(6)	2.164(6)	2.154(6)	2.134(9)
M2-O3	2.065(6)	2.059(5)	2.038(6)	2.033(5)	2.023(5)	2.018(5)	2.010(6)	1.997(6)	1.987(6)	1.987(9)
M2-O2	2.067(7)	2.044(6)	2.026(7)	2.024(6)	2.022(6)	2.012(6)	2.002(7)	1.980(7)	1.977(7)	1.983(11)
M2-O1	2.191(8)	2.172(6)	2.150(7)	2.131(6)	2.120(6)	2.115(6)	2.107(7)	2.085(7)	2.071(7)	2.056(11)
Average bond length (Å)	2.141(6)	2.130(6)	2.113(6)	2.103(5)	2.096(5)	2.089(5)	2.079(6)	2.064(6)	2.055(6)	2.047(8)
Polyhedral volume (Å ³)	12.56(1)	12.39(1)	12.12(1)	11.95(1)	11.83(1)	11.74(1)	11.59(1)	11.34(1)	11.21(1)	11.08(1)
Distortion indices (<i>D</i>)	0.03521	0.03559	0.03743	0.03468	0.03487	0.03482	0.0346	0.0355	0.03458	0.02992
SiO ₄ tetrahedron										
Si-O3	1.632(5)	1.639(5)	1.643(6)	1.634(5)	1.630(5)	1.632(5)	1.635(6)	1.622(6)	1.628(6)	1.620(9)
Si-O2	1.664(7)	1.655(5)	1.659(6)	1.655(5)	1.652(6)	1.655(5)	1.656(7)	1.650(7)	1.642(7)	1.639(10)
Si-O1	1.598(11)	1.608(8)	1.596(9)	1.596(8)	1.577(9)	1.584(8)	1.583(9)	1.574(10)	1.574(10)	1.565(15)
Average bond length (Å)	1.632(8)	1.635(5)	1.635(6)	1.630(5)	1.622(6)	1.626(5)	1.627(6)	1.617(7)	1.618(6)	1.611(10)
Polyhedral volume (Å ³)	2.194(8)	2.208(7)	2.209(8)	2.184(7)	2.155(7)	2.166(7)	2.170(8)	2.133(9)	2.135(9)	2.103(13)
Distortion indices (<i>D</i>)	0.01042	0.00829	0.01201	0.01025	0.01387	0.01285	0.0136	0.01327	0.01363	0.01431

polyhedra (Hazen and Finger 1979). The compressibility of the [MO₆] octahedra, which have longer bond lengths, plays a critical role in controlling the compressional behavior of olivine (Bass and Anderson 1984). Among the octahedra,

the [M2O₆] octahedron exhibits higher compressibility compared to the [M1O₆] octahedron (Fig. 8).

For the Mg-rich (Fo₇₇Fa₂₃) and Fe-rich (Fo₂₉Fa₇₁) olivine samples, the volume compressions of the [M2O₆] octahedra are comparable, approximately 0.084 Å³/GPa. In contrast,

Fig. 8 Average bond length (a) and polyhedral distortion indices (b) of $\text{Fo}_{29}\text{Fa}_{71}$ and $\text{Fo}_{77}\text{Fa}_{23}$ olivine under high pressure. The blue data points are referenced from Pamato et al. (2019)



the $[\text{M1O}_6]$ octahedra exhibit different compressions: $0.070 \text{ \AA}^3/\text{GPa}$ for $\text{Fo}_{77}\text{Fa}_{23}$ and $0.047 \text{ \AA}^3/\text{GPa}$ for $\text{Fo}_{29}\text{Fa}_{71}$. As Mg content increases, the bulk modulus decreases, indicating greater compressibility. Although the $[\text{M2O}_6]$ octahedra are more compressible, differences in the compressibility of Mg-Fe olivine with varying compositions are likely dominated by variations in the $[\text{M1O}_6]$ octahedra.

Compressional behavior is also reflected in distortion indices. Figure 8b illustrates the variation of polyhedral distortion indices with pressure. For both compositions, the distortion indices of the polyhedra exhibit minimal variation under increasing pressure. However, the $[\text{M2O}_6]$ octahedron consistently shows greater distortion, whereas the $[\text{SiO}_4]$ tetrahedron has a relatively low distortion indices. The $[\text{SiO}_4]$ tetrahedron is significantly less compressible than the $[\text{MO}_6]$ octahedra, which is consistent with our earlier findings (Fig. 8). A distinctive characteristic of silicate olivine under pressure is the rigidity and low compressibility of the $[\text{SiO}_4]$ tetrahedra, while the M1 and M2 octahedra undergo significant compression, controlling both the compressional behavior and anisotropy of olivine.

The ionic radius of Fe (78 pm) exceeds that of Mg (72 pm), indicating that Mg-O bonds are stronger than Fe-O bonds (Song 2009). This is reflected in the greater distortion of the $[\text{M1O}_6]$ and $[\text{M2O}_6]$ octahedra in $\text{Fo}_{29}\text{Fa}_{71}$ compared to $\text{Fo}_{77}\text{Fa}_{23}$. Furthermore, while the two Mg-O bonds of forsterite are almost totally ionic and equal in their degrees of ionicity, the Fe-O bonds of fayalite always display significant degrees of covalency (Fujino et al. 1981; Gonschorek 1986), which may account for the higher bulk modulus and lower compressibility of $\text{Fo}_{29}\text{Fa}_{71}$. However, this observation contrasts with the expected bond strength based solely on ionic radius considerations.

On the other hand, electronegativity also influences the ability of atoms to attract electrons. The electronegativity of Mg (1.31) is lower than that of Fe (1.83) (Allred 1961), suggesting that Fe exhibits stronger electron-attracting ability. This may contribute to differences in compressibility observed in olivine with varying Fe contents. Although Fe and Mg are nearly equally distributed between the M1 and

M2 sites without site preference based on our new structural refinements and previous analysis (Nestola et al. 2011; Pamato et al. 2019), the effects of Fe and Mg on compressibility cannot be attributed solely to differences in polyhedral distortion or average bond length. Nevertheless, the higher Fe content in $\text{Fo}_{29}\text{Fa}_{71}$ likely amplifies the influence of Fe's higher electronegativity, resulting in the lower compressibility of this composition.

Implication

The findings of this study have profound implications for understanding the elastic behavior of olivine in the Earth's upper mantle and its influence on geodynamic processes. The observed increase in bulk modulus with Fe content suggests that Fe-rich olivine is less compressible than its Mg-rich counterpart, which has direct consequences for seismic velocity profiles and mantle composition modeling. Since olivine is the dominant mineral in the upper mantle, its compressibility affects the interpretation of seismic wave speeds, particularly in regions with varying Fe/Mg ratios, such as subduction zones and mantle plumes (Abramson et al. 1997; Zha et al. 1998; Cammarano et al. 2010). The anisotropic compression behavior may also influence mantle anisotropy and deformation mechanisms, particularly through enhanced *b*-axis elongation and octahedral distortion caused by Fe incorporation. These effects provide insights into the development of lattice-preferred orientation (LPO) in mantle rocks (Zhang and Karato 1995).

Furthermore, the high rigidity of $[\text{SiO}_4]$ tetrahedra under compression, contrasted with the higher compressibility of $[\text{MO}_6]$ octahedra, indicates that the high-pressure behavior of olivine is governed mainly by changes in cation-oxygen bonding rather than by collapse of the silicate framework. This mechanistic insight suggests that phase transitions in the mantle transition zone, including the transformations of olivine to wadsleyite and ringwoodite, are controlled primarily by changes in cation coordination and not by the collapse of the silicate tetrahedra. The refined EoS parameters,

particularly the composition-dependent bulk modulus, improve the accuracy of thermodynamic modeling for mantle mineral assemblages, aiding in the prediction of phase stability boundaries and density variations.

Additionally, these results are critical for planetary science, as olivine is a key mineral in terrestrial planets and differentiated asteroids (Sanchez et al. 2014). The systematic relationship between Fe content and elasticity can help constrain the interior structures of Mars, Mercury, and exoplanetary mantles, where Fe-rich olivine may dominate (Isaak 1992; Speziale et al. 2004; Dumoulin et al. 2017). By bridging the gap between experimental mineral physics and geophysical observations, this study enhances our ability to decode mantle dynamics, from subduction zone processes to planetary evolution. Future work should extend these measurements to higher pressures and incorporate temperature effects to further refine mantle convection models.

Conclusion

This study systematically investigated the elastic properties and structural variations of synthetic Mg-Fe olivine solid solutions through synthetic sample preparation and high-pressure single-crystal XRD experiments. The results reveal that Fe incorporation has a pronounced influence on some of the unit-cell parameters, notably elongating the *b*-axis while leaving the *a*-axis largely unchanged. Structural refinements showed that increasing Fe content leads to elongation of the M1-O and M2-O bond lengths, with Fe and Mg distributed nearly equally between the M1 and M2 sites. In contrast, the Si-O bond lengths and tetrahedral structures exhibit negligible changes, maintaining their structural rigidity. By fitting the third-order Birch-Murnaghan EoS to pressure-volume data, this study determined that the bulk modulus exhibits a nonlinear increase with Fe content, ranging from 118 to 124 GPa, while the first pressure derivative K'_0 varies between 4.2 and 4.58.

High-pressure compression experiments further reveal that the [M2O₆] octahedra are more compressible than the [M1O₆] octahedra, while the [SiO₄] tetrahedra maintain their rigidity with minimal compressibility. Variations in compressibility across compositions are predominantly attributed to changes in the [M1O₆] octahedra, with Fe incorporation enhancing octahedral distortions in both [M1O₆] and [M2O₆] structures. Moreover, the higher electronegativity and ionic radius of Fe contribute to reduce compressibility and an increased bulk modulus in Fe-rich compositions. Additionally, the results contribute valuable constraints on the internal structure and evolutionary processes of Earth and other terrestrial planets.

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Author contributions Z.Y., J.X., and D.F. designed the project. Z.Y., J.X., D.F., D.Z., and W.Z. participated in the data collection and analysis. Z.Y. and J.X. were responsible for data interpretation and wrote the manuscript. D.F., D.Z., W.L., and W.Z. participated in the discussion and provided comments on the manuscript.

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Data availability No datasets were generated or analysed during the current study.

Declarations

Conflict of interest The authors declare no competing interests.

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