Structure, crystal chemistry, and compressibility of iron-rich silicate perovskite at pressures up to 95 GPa.

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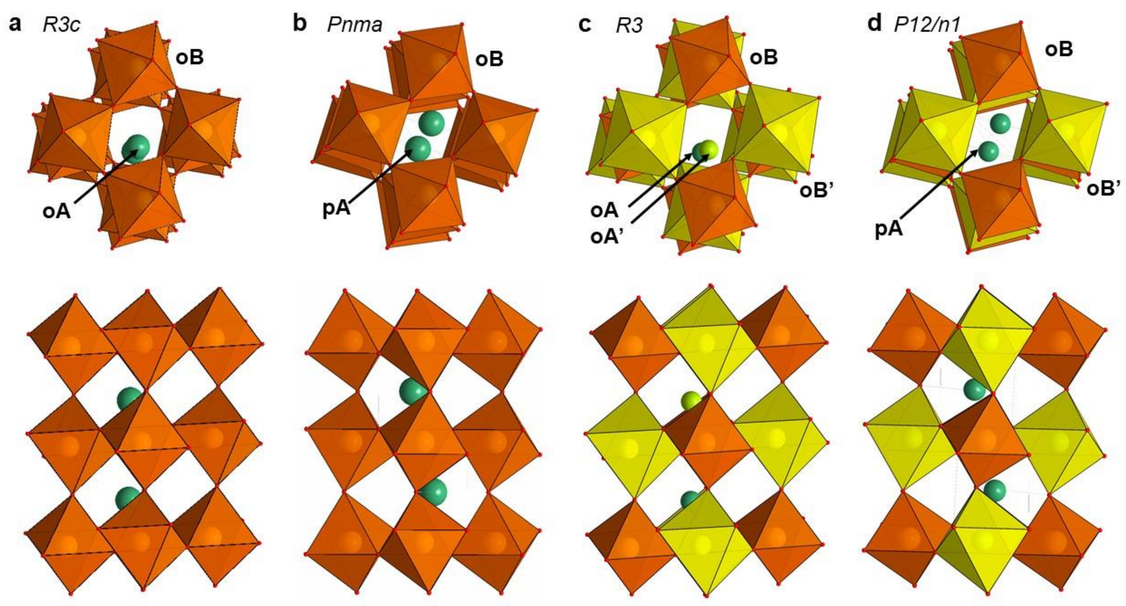
1. Introduction

Bridgmanite elasticity is influenced by chemical composition, oxygen vacancies, and pressure-induced high-spin to low-spin transition in iron. The effect of pressure-driven spin transition(s) in iron-bearing bridgmanite on bulk modulus is complex, because iron could occupy different crystallographic sites and can occur as both ferrous and ferric. In addition, high-pressure experiments with silicate perovskite end-members could provide us with a self-consistent elasticity database and clarify mechanism(s) of cations substitution.

2. Methods

Samples synthesis in Large Volume Press, diamond anvil cells for pressure generation, synchrotron radiation based *in situ* single-crystal X-ray diffraction, and Mössbauer spectroscopy.

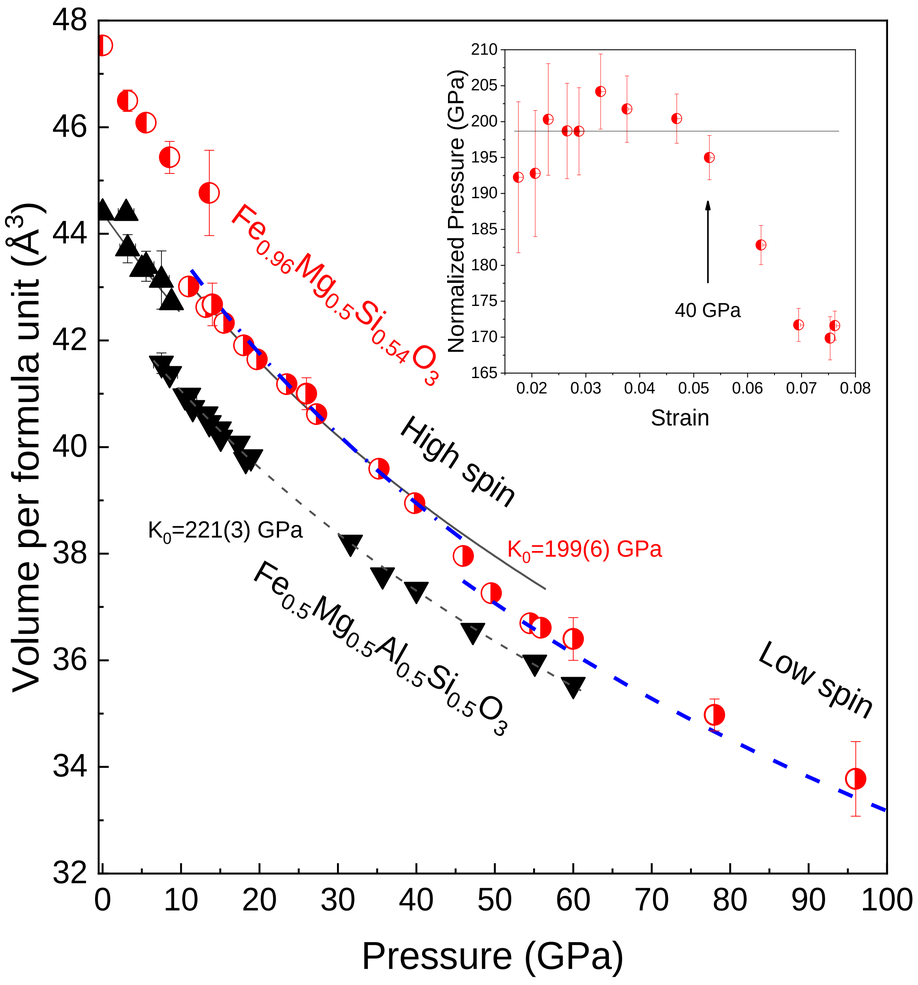
3. Results: Structures and their relations



Crystal structures of $Fe_{0.5}Mg_{0.5}Al_{0.5}Si_{0.5}O_3$ (a, b) and $Fe_{0.96}Mg_{0.5}Si_{0.54}O_3$ (c, d) silicate phases and their structural relations

(a,c) Phases stable at P<10 GPa, (b,d) Phases stable at P>10 GPa. Distinguishable crystallographic sites are different in color. pA refers to prismatic A-site, oB and oB' refers to octahedral B- and B'-site

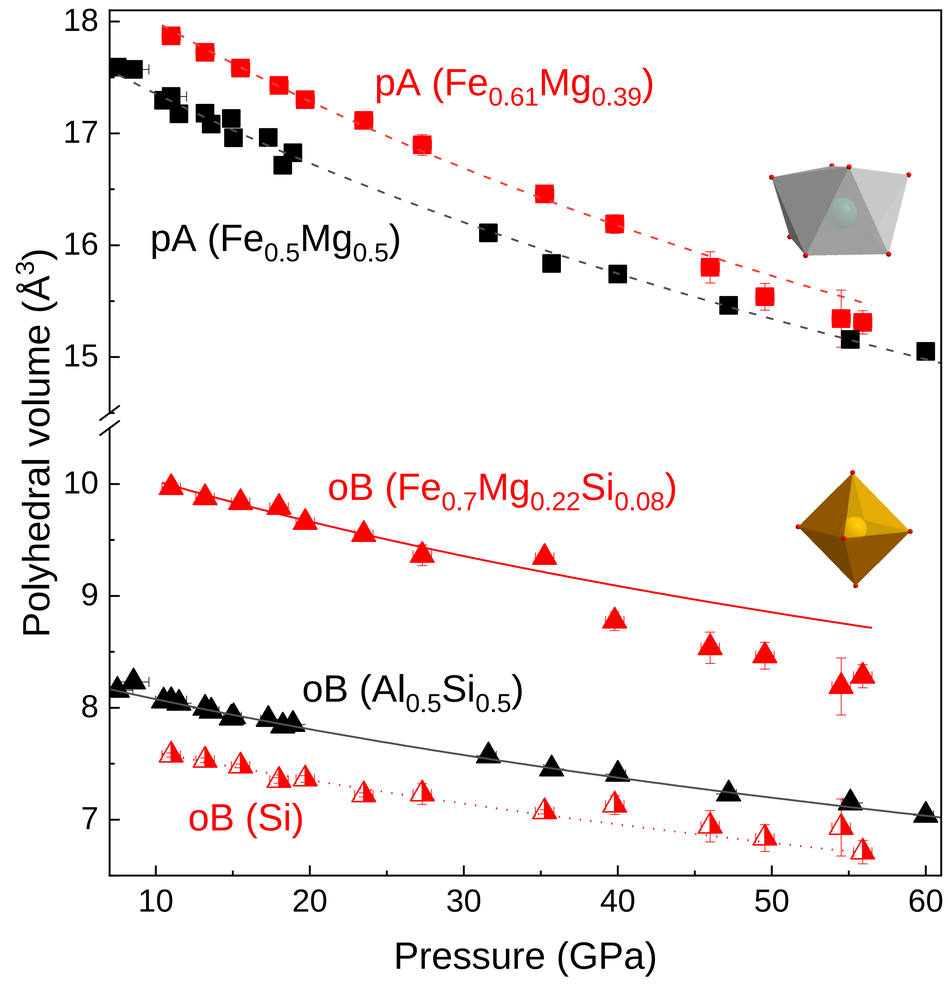
4. Results: Compressibility



Cold compression behaviour of $Fe_{0.5}Mg_{0.5}Si_{0.5}Al_{0.5}O_3$ and $Fe_{0.96}Mg_{0.5}Si_{0.54}O_3$

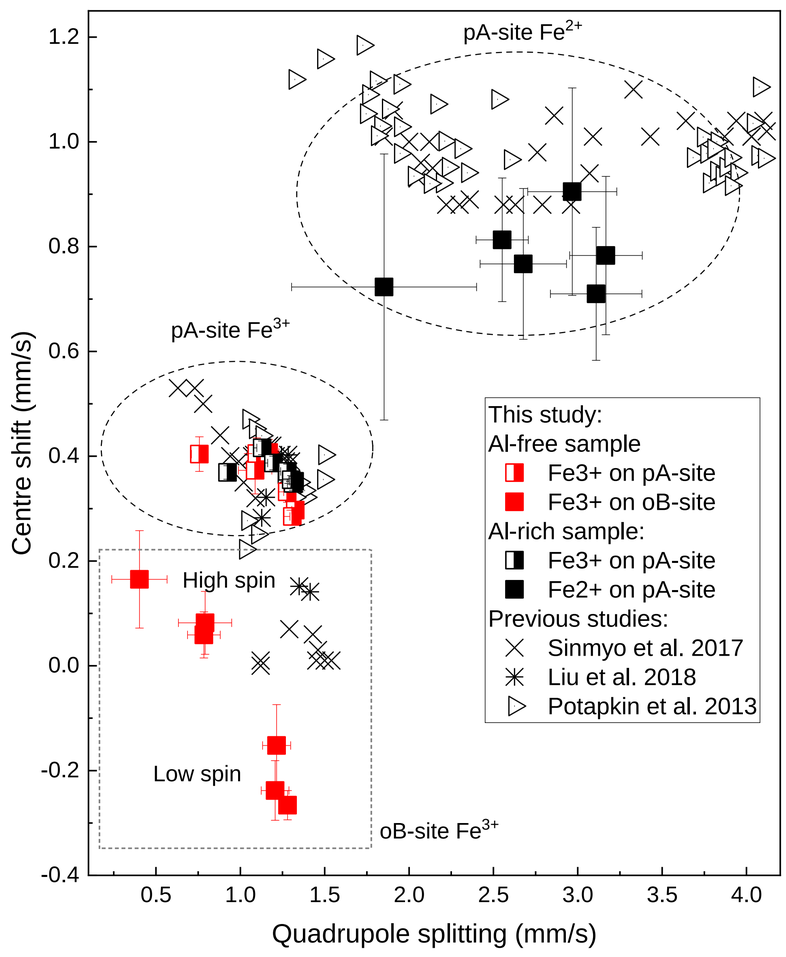
Black lines represent fits of P-V data with second order Birch-Murnaghan EoS. Blue lines are data from (Lin et al., 2000).At pressures above ~10 GPa samples with both compositions transform to (pseudo) orthorhombic perovskite-type structured phases. Inset: Above 40 GPa softening of the phase is obvious and related to spin transition of Fe^{3+} located in the B'-site of double-perovskite.

5. Results: Crystal chemistry



Compressibility of individual polyhedra in Al-rich silicate perovskite (black) and Al-poor silicate double perovskite (red).

6. Results: Mössbauer spectroscopy



A summary of quadrupole splitting and centre shift of silicate perovskite samples at high pressure.

For comparison, we plotted data from previous studies involving data collection on Fe-bearing bridgmanites. **Liu et al. 2018** (stars) used nuclear forward scattering; **Sinmyo et al. 2017** (crosses) and **Potapkin et al. 2013** (triangles) used SMS.

Key points:

- *First silicate double-perovskite*
- *New corundum-structure derivative*
- *Fe,Mg-bearing octahedral site in dPv*