

Crystal chemistry and compressibility of $\text{Fe}_{0.5}\text{Mg}_{0.5}\text{Al}_{0.5}\text{Si}_{0.5}\text{O}_3$ and $\text{FeMg}_{0.5}\text{Si}_{0.5}\text{O}_3$ silicate perovskites at pressures up to 95 GPa.

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Bridgmanite is widely considered the most abundant mineral in the Earth's lower mantle. Its properties control the dynamics of this region and a large number of previous studies have been focused on the behaviour of bridgmanite at mantle conditions. Bridgmanite elasticity may be affected by chemical variations, presence of oxygen vacancies, and pressure-induced high-spin to low-spin transition in iron. In the case of bridgmanite, the effect of pressure-driven spin transitions on bulk modulus is complex, because iron could occupy different crystallographic sites and can occur as both ferrous and ferric iron. In addition, high-pressure experiments with silicate perovskite end-members could provide us with a self-consistent elasticity database and clarify spin transition impact on elasticity.

We investigate crystalline materials with two compositions, $\text{FeMg}_{0.5}\text{Si}_{0.5}\text{O}_3$ and $\text{Fe}_{0.5}\text{Mg}_{0.5}\text{Al}_{0.5}\text{Si}_{0.5}\text{O}_3$, recovered after experiments in Kawai-type multi-anvil apparatus. After full sample characterization in terms of chemical composition, crystal structure, and iron oxidation state, we performed a series of compressibility experiments in diamond anvil cells up to 95 GPa. During compression, we collected single crystal X-ray diffraction patterns as well as Mössbauer spectra, which allowed us to follow up changes in crystal chemistry and Fe spin state during compression.

Our compressibility study on the Al-rich sample together with previously published data allowed us to reconstruct FeAlO_3 end-member compressibility. We found that $\text{FeMg}_{0.5}\text{Si}_{0.5}\text{O}_3$ has a previously unknown structure: the low-pressure phase is corundum-related type (space group $R\bar{3}$), and above about 15 GPa it transforms to a new silicate double-perovskite. An outstanding feature of the silicate double perovskite structure is two individual octahedral sites; one occupied by Si only, and the other by iron and magnesium. Combining single crystal X-ray diffraction data and results of Mössbauer spectroscopy, we were able to decipher the crystal chemistry behaviour of this phase during iron spin crossover, which is detectable by both compressibility changes of individual polyhedra and variation of Mössbauer hyperfine parameters.

Keywords: silicate perovskite, single crystal X-ray diffraction, Mössbauer spectroscopy