A synchrotron Mössbauer spectroscopy study of (Mg,Fe)SiO₃ perovskite up to 120 GPa

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ABSTRACT

The electronic environment of the Fe nuclei in two silicate perovskite samples, $Fe_{0.05}Mg_{0.95}SiO_3$ (Pv05) and $Fe_{0.1}Mg_{0.9}SiO_3$ (Pv10), have been measured to 120 GPa and 75 GPa, respectively, at room temperature using diamond anvil cells and synchrotron Mössbauer spectroscopy (SMS). Such investigations of extremely small and dilute ⁵⁷Fe-bearing samples have become possible through the development of SMS. Our results are explained in the framework of the "three-doublet" model, which assumes two Fe²⁺-like sites and one Fe³⁺-like site that are well distinguishable by the hyperfine fields at the location of the Fe nuclei. At low pressures, Fe³⁺/ Σ Fe is about 0.40 for both samples. Our results show that at pressure extending into the lowermost mantle the fraction of Fe³⁺ remains essentially unchanged, indicating that pressure alone does not alter the valence states of iron in (Mg,Fe)SiO₃ perovskite. The quadrupole splittings of all Fe sites first increase with increasing pressure, which suggests an increasingly distorted (noncubic) local iron environment. Above pressures of 40 GPa for Pv10 and 80 GPa for Pv05, the quadrupole splittings are relatively constant, suggesting an increasing resistance of the lattice against further distortion. Around 70 GPa, a change in the volume dependence of the isomer shift could be indicative of the endpoint of a continuous transition of Fe³⁺ from a high-spin to a low-spin state.