Local structure variations observed in orthoenstatite at high pressures

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ABSTRACT

The site-specific behavior of iron in an orthoenstatite-structured ⁵⁷Fe-enriched (M1)(M2)Si₂O₆ powdered sample was explored using synchrotron Mössbauer spectroscopy and diamond-anvil cells in two independent experiments at ambient temperature. In one experiment, NaCl was used as the pressure-transmitting medium (ambient pressure to 36 GPa), and in the other experiment, Ne surrounded the sample (4.1 to 26.8 GPa). The hyperfine parameters of the M1 and M2 sites at room pressure are in excellent agreement with previous literature values obtained using conventional Mössbauer spectroscopy and yield (Mg_{0.980}Fe_{0.020(5)})(Mg_{0.760}Fe_{0.240})Si₂O₆ as the chemical formula. Analyses of both data sets reveal a change in the trend or discontinuity in the hyperfine parameters around 10 GPa, indicative of a transformation in orthopyroxene. However, the detailed behaviors of the iron sites with pressure appear to depend on the local stress conditions provided by the different pressure media. Our observations may help explain the reported variations in structural transition behavior for orthopyroxenes at high pressures.

Keywords: Orthoenstatite, pyroxene, upper mantle, Mössbauer spectroscopy, nuclear resonant scattering