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High-resolution synchrotron X-ray powder diffraction and Rietveld structure refinement of two $(Mg_{0.95},Fe_{0.05})SiO_3$ perovskite samples synthesized under different oxygen fugacity conditions

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ABSTRACT

This paper presents high-resolution synchrotron X-ray powder diffraction data at 290 K on two Fe-bearing, polycrystalline silicate perovskite samples with approximate compositions $(Mg_{0.95}Fe_{0.05})SiO_3$ synthesized at 25 GPa and 1920 K in a multi-anvil press at different oxygen fugacity conditions. Mössbauer studies have indicated that $Fe^{3+}/\Sigma Fe$ for the samples are 0.09 ± 0.01 and near 0.16 ± 0.03. Rietveld structural refinements confirm that Fe^{2+} and Fe^{3+} dominantly substitute for Mg^{2+} in the 8-fold to 12-fold coordinated A site for both compositions. There appears to be no significant differences in the bond distances for these amounts of Fe^{3+} and no conclusive structural evidence to support indications from Mössbauer experiments that Fe^{3+} may occupy both A and B sites. To explore the effect of valence state further, this study also reports the first diffraction patterns of $(Mg,Fe)SiO_3$ perovskite collected at a wavelength near the Fe absorption edge.