

In situ structure determination of the high-pressure phase of Fe₃O₄

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ABSTRACT

The crystal structure of a high-pressure Fe₃O₄ phase was determined by in situ X-ray diffraction measurements at high pressure and temperature, using an imaging plate detector and monochromatic synchrotron X-radiation. The high-pressure phase has the *Pbcm* space group (CaMn₂O₄-type structure) with cell parameters $a = 2.7992(3)$ Å, $b = 9.4097(15)$ Å, and $c = 9.4832(9)$ Å at 23.96 GPa and 823 K. Fe³⁺ occupies an octahedral site and Fe²⁺ is in an eightfold-coordinated site described as a bicapped trigonal prism. The high-pressure CaMn₂O₄-type Fe₃O₄ phase is about 6.5% more dense than the spinel form at 24 GPa.