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High-pressure and high-temperature phase transitions in $FeTiO_3$ and a new dense $FeTi_3O_7$ structure

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Abstract

High-pressure and high-temperature phase relations of $FeTiO_3$ were investigated up to a pressure of about 74 GPa and 2600 K by synchrotron X-ray diffraction and analytical transmission electron microscopy. We conclude that $FeTiO_3$ ilmenite transforms into the following phase(s) with increasing pressure: $FeTiO_3$ (perovskite) at 20–30 GPa, Fe_2TiO_4 (Ca_2TiO_4-type) + TiO_2 (OI-type) at 30–44 GPa and high temperature, FeO (wüstite) + TiO_2 (OI) at 30–44 GPa and low temperature, and wüstite + $FeTi_3O_7$ (orthorhombic phase) above 44 GPa. Among these dense high-pressure polymorphs, $FeTi_3O_7$ is a new compound and its structure analysis was tried using particle swarm optimization simulation. This method successfully found a new high-density $FeTi_3O_7$ structure, and Rietveld refinement based on this model structure gave an excellent fit with the experimentally obtained X-ray diffraction pattern. This new high-density $FeTi_3O_7$ structure consists of polyhedra for monocapped FeO_7 prisms, bicapped TiO_8 prisms, and tricapped TiO_9 prisms, which develop on the **b-c** plane and stack along the **a** axis. The dense compound assemblage found in $FeTiO_3$ is promising for investigating the behavior of ABX_3 compounds under ultrahigh pressures.

Keywords: $FeTiO_3$, $FeTi_3O_7$, high pressure, diamond-anvil cell