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SPINELS RENAISSANCE: THE PAST, PRESENT, AND FUTURE OF THOSE UBIQUITOUS MINERALS AND MATERIALS

New structure of high-pressure body-centered orthorhombic Fe_2SiO_4†

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Abstract

A structural change in Fe_2SiO_4 spinel (ringwoodite) has been found by synchrotron powder diffraction study and the structure of a new high-pressure phase was determined by Monte-Carlo simulation method and Rietveld profile fitting of X-ray diffraction data up to 64 GPa at ambient temperature. A transition from the cubic spinel structure to a body centered orthorhombic phase (I-Fe_2SiO_4) with space group *Imma* and $Z = 4$ was observed at approximately 34 GPa. The structure of I-Fe_2SiO_4 has two crystallographically independent FeO_6 octahedra. Iron resides in two different sites of sixfold coordination: Fe1 and Fe2, which are arranged in layers parallel to (101) and (011) and are very similar to the layers of FeO_6 octahedra in the spinel structure. Silicon is located in the sixfold coordination in I-Fe_2SiO_4. The transformation to the new high-pressure phase is reversible under decompression at ambient temperature. A martensitic transformation of each slab of the spinel structure with translation vector $\langle \overrightarrow{1/8}\ \overrightarrow{1/8}\ \overrightarrow{1/8} \rangle$ generates the I-Fe_2SiO_4 structure. Laser heating of I-Fe_2SiO_4 at 1500 K results in a decomposition of the material to rhombohedral FeO and SiO_2 stishovite.

Fe$K\beta$ X-ray emission measurements at high pressure up to 65 GPa show that the transition from a high spin (HS) to an intermediate spin (IS) state begins at 17 GPa in the spinel phase. The IS electron spin state is gradually enhanced with pressure. The Fe^{2+} ion at the octahedral site changes the ion radius under compression at the low spin, which results in the changes of the lattice parameter and the deformation of the octahedra of the spinel structure. The compression curve of the lattice parameter of the spinel is discontinuous at ~20 GPa. The spin transition induces an isostructural change.

Keywords: New high-pressure structure, Fe_2SiO_4 ringwoodite, X-ray emission spectra, spin transition, martensitic transition