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Fe2SiO4 スピネル相（Ringwoodite 端成分）の新高圧と構造と 高圧下での電子スピン状態変化
A new high pressure phase of Fe2SiO4 and the relationship between spin and structural transitions

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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 six-fold coordination: Fe1 and Fe2, which are arranged in layers parallel to (101) and (011), and very similar to the layers of FeO_6 octahedra in the spinel structure. Silicon is located in the six-fold 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 transition vector <1/8 1/8 1/8 >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 65GPa 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 Fe2+ ion at the octahedral site changes the iron radius under compression from 0.78 A at the high-spin state to 0.61 A 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 approximately 20 GPa. The spin transition induces an isostructural change.

キーワード: Fe2SiO4 スピネル, 新高圧体心斜方賞構造, スピン転移, X?線エミッション, マルテンサイト転移
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