

Structure change of MgSiO₃, MgGeO₃, and MgTiO₃ ilmenites under compression

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ABSTRACT

Compression mechanisms of A²⁺B⁴⁺O₃ ilmenites with compositions MgSiO₃ (stable at high pressures), MgGeO₃ (stable at moderate pressures), and MgTiO₃ (stable at ambient pressure) were investigated at high pressure by single-crystal structure analysis, using both synchrotron radiation and an MoK α rotating-anode X-ray generator. The distortions of AO₆ (A:Mg) and BO₆ (B: Si,Ge,Ti) octahedra under pressure were parameterized by bond length, shared-face area, site-volume ratio, and A²⁺-B⁴⁺ interatomic distance across the shared edges and shared face. The AO₆ octahedral volume is much more compressive than the BO₆ octahedral volume. Of the three samples, both the AO₆ and BO₆ octahedra are most rigid in MgSiO₃. The A²⁺-B⁴⁺ interatomic distance becomes more shortened with increasing pressure than do the A²⁺-A²⁺ and B⁴⁺-B⁴⁺ distances. The compression of Mg-Si is more remarkable than that of Mg-Ge and Mg-Ti. The A-B interatomic distance along **c** is more compressed with increasing pressure than A-A and B-B along **a**. The short A-B distance across the shared face becomes more shortened than the A-A and B-B distances across the shared edge. The cation position moves in the direction of **c** with pressure and tends to approach the center of the AO₆ and BO₃ octahedra with increasing pressure. The regularity of the octahedra is enhanced at higher pressure. Both quadratic elongation and bond angle variance verify the reduction of the deformation of AO₆ and BO₆ octahedra with pressure.