Single-crystal X-ray diffraction of grunerite up to 25.63 GPa: A new high-pressure clinoamphibole polymorph

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Abstract

High-pressure single-crystal X-ray diffraction experiments were conducted on natural grunerite crystals using a synchrotron X-ray source with composition $(Fe_{5.237}Mg_{1.646}Ca_{0.061}Mn_{0.051}Na_{0.015})(Si_{7.932}Al_{0.083})O_{22}(OH)_2$. Grunerite has *C*2/*m* symmetry at ambient conditions. The samples were compressed at 298 K in a diamond-anvil cell to a maximum pressure of 25.6(5) GPa. We observe a previously described phase transition from *C*2/*m* (α) to $P2_1/m$ (β) to take place at 7.4(1) GPa, as well as a further transition from $P2_1/m$ (β) to *C*2/*m* (γ) at 19.2(3) GPa. The second-order Birch-Murnaghan equation of state fit to our compressional data, yielded the values V_0 = 914.7(7) Å^3 and K_0 = 78(1) GPa for α-grunerite, V_0 = 926(5) Å^3 and K_0 = 66(4) GPa for β-grunerite and V_0 = 925(27) Å^3 and K_0 = 66(13) GPa for γ-grunerite. The β – γ phase transition produces a greater degree of kinking in the double silicate chains of tetrahedra accompanied by a discontinuous change in the a and c unit cell parameters and the monoclinic β angle. At 22.8(4) GPa the O5-O6-O5 kinking angle of the new high-pressure *C*2/*m* phase is 137.5(4)°, which is the lowest reported for any monoclinic amphibole. This study is the first structural report to show the existence of three polymorphs within an amphibole group mineral. The high-pressure γ-phase illustrates the parallel structural relations and phase transformation behavior of both monoclinic single and double chain silicates.