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Compressibility of protoamphibole: A high-pressure single-crystal diffraction study of protomangano-ferro-anthophyllite

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Abstract

The high-pressure behavior of protoamphibole (space group *Pnmn*) was studied by in situ single-crystal X-ray diffraction on a sample of protomangano-ferro-anthophyllite with formula $(Mn_{1.39}Fe_{0.59})(Fe_{3.98}Mg_{1.02})Si_8O_{22}(OH)_2$, from Yokone-Yama, Awano Town, Tochigi Prefecture, Japan. Unit-cell parameters were collected at various pressures up to 9 GPa, and structural refinements were obtained from data collected at several pressures up to 7 GPa. Fitting the *P*-*V* data to a third-order Birch-Murnaghan equation of state (EoS) gives the following parameters: K_{T0} = 64(1) GPa, K' = 7.0(4), and V_0 = 926.4(4) Å^3. Axial moduli are: K_{0a} = 30.7(8) GPa, K'_a = 10.8(5), and a_0 = 9.430(2) Å; K_{0b} = 109(4) GPa, K'_b = 2.7(8), and b_0 = 18.364(4) Å; K_{0c} = 94(5), GPa, K'_c = 4(1), and c_0 = 5.354(2) Å. The corresponding axial compressibilities (10^{-3} GPa^{-1}) are β_a = 10.9(3), β_b = 3.1(1), and β_c = 3.5(2), and indicate that the HP behavior of protomangano-ferro-anthophyllite is highly anisotropic, the highest compressibility being along [100]. No discontinuous behavior or polymorphic transitions were observed in the pressure range studied.

Structural refinements show that M1, M2, and M3 polyhedra have similar compressibilities, owing to their similar composition. M4 (72% Mn, 28% Fe) is a highly distorted site and is slightly softer than the other octahedra. The major movements in the tetrahedral ribbon concern kinking of the double chain, bending along the [100] direction through the empty A site, and tetrahedral rotation, necessary to maintain coherence with the octahedral layer. The kinking angle of O5-O6-O5, which in air is 179.1(2)°, decreases to 174(2)° at 6.9 GPa. The T1-O7-T1 angle changes from 143.8(3)° to 134(5)° at 6.9 GPa, and the tetrahedral rotation α increases from 0.2(2)° to 4(2)°.

Keywords: Protoamphibole, protomangano-ferro-anthophyllite, compressibility, equation of state, high-pressure structure