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The effect of oxo-component on the high-pressure behavior of amphiboles

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Abstract

The role of the oxo-component on the compressibility of amphibole was studied by means of high-pressure in situ single-crystal X-ray diffraction on two natural kaersutite megacrysts (samples DL5 and FR12) from alkaline basalts. The oxo-component varies significantly (1.1 and 1.9 apfu in DL5 and FR12, respectively), whereas the cation composition is very similar, apart from the $Fe^{3+}/(Fe^{2+}+Fe^{3+})$, which is 0.33 in DL5 and ~1 in FR12. The larger oxo-component of FR12 is attributed to the $Fe^{2+} + OH^{-} = Fe^{3+} + O^{2-} + ½H_2$ substitution.

Unit-cell parameters were collected at different pressures up to about 8 GPa. Structural refinements of both samples were performed with data collected at different P up to 6 GPa. Fitting the P-V data to a third-order Birch Murnaghan EoS yielded the following parameters: $K_0 = 94(1)$ GPa, $K' = 6.3(4)$, and $V_0 = 903.6(2)$ Å^3 for FR12 and $K_0 = 91(2)$ GPa, $K' = 6.2(4)$, and $V_0 = 914.1(2)$ Å^3 for DL5. The axial moduli of the two amphibole samples were: $K_{0a} = 86(3)$ GPa, $K'_a = 7(1)$, and $a_0 = 9.815(2)$ Å; $K_{0b} = 115(3)$ GPa, $K'_b = 4.8(8)$, and $b_0 = 18.012(2)$ Å; $K_{0c} = 112(5)$ GPa, $K''_c = 7(1)$, and $c_0 = 5.300(1)$ Å for sample FR12 and $K_{0a} = 85(3)$ GPa, $K'_a = 5(1)$, and $a_0 = 9.8660(9)$ Å; $K_{0b} = 113(2)$, $K'_b = 4.4(6)$, and $b_0 = 18.0548(6)$ Å; $K_{0c} = 107(3)$ GPa, $K'_c = 7(1)$, and $c_0 = 5.3185(5)$ Å for sample DL5. This suggests that the compressibility of kaersutite decreases with increasing oxo-component.

Structural refinements show that the polyhedral compressibility follows the order A = M4 > M2 > M3 > M1 for DL5 and A = M4 > M2 > M1 > M3 for FR12. The most evident geometrical effect induced by P is the decrease in the bending of the double tetrahedral chain, when adjacent I-beams are pushed against each other. This effect is largest for DL5, which has a larger concavity of the A site, (O7-O7′ changes from 3.03 to 2.82 Å) compared to the one of FR12, (O7-O7′ changes from 2.92 to 2.79 Å). This mechanism is confirmed by the evolution of T1-O7-T1 angle (from 135.4° to 132.5° in FR12 and from 136.6° to 132.2° in DL5).

Keywords: Oxo-amphiboles, kaersutite, compressibility, equation of state, high-pressure structure, amphibole