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High-pressure phase transition of a natural pigeonite

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Abstract

High-pressure and room-temperature single-crystal X-ray diffraction (XRD) studies have been performed on crystals of a natural pigeonite sample with composition ca. $Wo_{10}En_{43}Fs_{47}$ using diamond-anvil cells. The unit-cell parameters were determined at 18 different pressures up to about 6 GPa. A first-order $P2_1/c$-$C2/c$ phase transition was found between 3.5 and 3.6 GPa, associated with the disappearance of the *b*-type reflections ($h + k$ = odd) and a strong discontinuity (about 1.7%) in the unit-cell volume. At the transition, a small hysteresis (~0.3 GPa) was observed. A third-order Birch-Murnaghan equation of state (BM3-EoS) fit to the 10 *P*-*V* data of the low-*P* phase yielded V_0 = 431.93(2) Å^3, K_{T0} = 96.8(8) GPa and K' = 8.5(6). A second-order Birch-Murnaghan EoS fit to the 8 *P*-*V* data (between 3.6 and 6 GPa) of the *C*2/*c* high-*P* phase yielded V_0 = 423.6(1) Å^3 and K_{T0} = 112.4(8), indicating that the high-*P* *C*2/*c* phase is significantly stiffer than the low-*P* phase.

In a separated experiment with crystals of the same sample, intensity data were collected and crystal structures were refined at 13 pressures up to 9.4 GPa. The M1-O and M2-O mean bond lengths of the low-*P* $P2_1/c$ phase decrease by 0.7 and 2.1%, respectively. The two non-equivalent A and B tetrahedral chains become more kinked with pressure, with a reduction of their angle by 2.2 and 5.1%, respectively. At the transition the A-chain changes sense of rotation and both chains become equivalent and more kinked, with a further reduction of their angle by 2.5% up to 9.4 GPa.

Strain calculations have been performed and the evolution of the spontaneous strain and the order parameter variation with pressure are discussed, considering geometrical parameters of the structure and comparing our results with the available data for other compositions.

Keywords: Pigeonite, high-pressure, single crystal XRD, diamond-anvil cell, phase transition, spontaneous strain