American Mineralogist, Volume 100, pages 1568–1577, 2015

High-pressure equation of state and phase transition in $PbAl_2Si_2O_8$ feldspar

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Abstract

In situ high-pressure X-ray diffraction study was performed on synthetic lead feldspar with composition $PbAl_2Si_2O_8$ (PbFsp). The crystals were synthesized from the melt and thermally treated at $T = 1150$ °C for 12 h and at $T = 1000$ °C for 70 h. At room condition the unit-cell parameters are $a = 8.3936(4)$, $b = 13.0498(7)$, $c = 14.3258(8)$ Å, $\beta = 115.281(6)°$, $V = 1418.9(1)$ Å^3; space group: $I2/c$; $Q_{od} = 0.7$.

A single-crystal of lead feldspar was loaded in an ETH-type diamond-anvil cell and unit-cell parameters were measured at 26 different pressures up to 8.4 GPa at room *T*. The evolution with *P* of the unit-cell parameters and volume shows a strong discontinuity between 7.7 and 8.2 GPa indicating a first-order phase transition. The discontinuous character of the transition is especially noticeable in the behavior of the β angle, which decreases from 114.83° to 114.03°, and in the *b* parameter, which reduces from 12.746 to 12.567 Å.

In the *P* range 0.0001–7.72 GPa, the trend shown by the axial compressibility ($\beta_a > \beta_c > \beta_b$) is similar to that observed in the previous HP powder diffraction study, performed on lead feldspar using high-brilliance synchrotron radiation up to 7.1 GPa.

In the *P* range 0.0001–4.27 GPa at room *T*, the *P*-*V* data of the *I*2/*c* lead feldspar were fitted with a second-order Birch-Murnaghan EoS. The parameters obtained are: $V_0 = 1422.2(1)$ Å^3 and $K_{T0} = 76.4(9)$ GPa. At $P > 4.27$ GPa, the volume values deflect from the BM2 curve and show a volume softening, precursor of the reported HP phase transition. A volume softening was recently observed in strontium feldspar (SrFsp) above 4.2 GPa.

A second crystal of PbFsp was loaded in the DAC cell and in situ high-pressure X-ray diffraction intensities were measured at $P = 0.0001$, 2.4, 3.1, 5.4, 6.0, 7.2, 8.4, and 9.7 GPa. The appearance of *c* and *d*-type reflections at 8.4 GPa, the analysis of the systematic absence and the structural refinements indicate the HP first-order transformation as an $I2/c$-$P2_1/c$ phase transition. Structural results show that the main variations with compression in lead feldspar are in Pb-O bond lengths and in T-O-T bond angles, while T-O distances and O-T-O angles do not change meaningfully, indicating that the Si,Al tetrahedra behave with pressure as a rigid body. Changes observed in the compressional behavior of the structure between 3 and 5 GPa could explain the softening observed at $P > 4$ GPa in the volume compressibility.

The results obtained in the present work allow comparing the pressures of the HP $I2/c$-$P2_1/c$ phase transition occurring in lead feldspar with those observed in alkaline-earth feldspars.

Keywords: Crystal structure, high-pressure studies, lead feldspar, equation of state, phase transition