High-pressure equation of state and phase transition in PbAl$_2$Si$_3$O$_8$ feldspar

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ABSTRACT

In situ high-pressure X-ray diffraction study was performed on synthetic lead feldspar with composition PbAl$_2$Si$_3$O$_8$ (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, $\beta = 115.281(6)^\circ$, $V = 1418.9(1)$ Å$^3$; space group: $I2/c$; $Q_{el} = 0.7$.

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 $\beta$ 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 ($\beta_a > \beta_b > \beta_c$) 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 $I2/c$ lead feldspar were fitted with a second-order Birch-Murnaghan EoS. The parameters obtained are: $V_0 = 1422.2(1)$ Å$^3$ and $K_{0p} = 76.4(9)$ 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

INTRODUCTION

Several studies were performed on natural and synthetic feldspars to investigate their equations of state (EoS) and symmetry changes with pressure; however, taking into account the complexity of their potential chemical and structural arrangements, the number of high-quality data available in literature remains still limited. In a review on the behavior of feldspars at high-pressure conditions, Angel (1994) and Ross (2000) observed that the tetrahedra of the framework behave like almost a rigid body and the main compressional mechanism is the T-O-T bond bending. The degree of Al, Si order influences the HP elastic behavior of feldspars and, in particular, an increase of Al, Si disorder results in a small decrease in bulk modulus (Angel et al. 1988; Angel 1994; Downs et al. 1994; Allan and Angel 1997; Benusa et al. 2005; Sochalski-Kolbus et al. 2010; Curetti et al. 2011b).

In feldspars with Al:Si ratio equal to 1:1, the symmetry at room condition is determined by the non-tetrahedral M cation: triclinic $P\overline{1}$ (or $I\overline{1}$) space group is observed when the M-site is occupied by Ca (anorthite, CaAl$_2$Si$_2$O$_8$), An, Megaw et al. (1962), monoclinic $I2/c$ symmetry when the M-site is occupied by a larger cation as Sr, Pb, Ba (strontium feldspar, SrAl$_2$Si$_2$O$_8$, SrFsp, Chiari et al. 1975; lead feldspar, PbAl$_2$Si$_2$O$_8$, PbFsp, Bruno and Facchinelli 1972; BaAl$_2$Si$_2$O$_8$, celsian, Newman and Megaw 1960). Along the anorthite-strontium feldspar (An-SrFsp) join at ambient conditions, the structure of feldspars changes with composition from $P\overline{1}$ to $I2/c$, through an intermediate $I\overline{1}$ structure. The $P\overline{1}$-$I\overline{1}$ phase transition occurs near An$_{50}$SrFsp$_{50}$ composition (Phillips et al. 1997; Tribaudino et al. 2000, 2005) and the $I\overline{1}$-$I2/c$ zone-center displacive ferroelastic transition, strongly affected by different Al, Si order (Tribaudino et al. 1993, 2009), was observed near An$_{10}$SrFsp$_{90}$ in ordered feldspars (Bambauer and Nager...