The high-pressure structural configurations of Ca<sub>0.2</sub>Sr<sub>0.8</sub>Al<sub>2</sub>Si<sub>2</sub>O<sub>8</sub> feldspar: The $\overline{1}$-12/c and 12/c-P2<sub>1</sub>/c phase transitions

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ABSTRACT

Single-crystal in situ high-P X-ray diffraction was performed at $P = 0.0001$, 3.2, 4.4, 6.2, and 7.4 GPa on synthetic Ca<sub>0.2</sub>Sr<sub>0.8</sub>Al<sub>2</sub>Si<sub>2</sub>O<sub>8</sub> (An<sub>20</sub>SrF<sub>80</sub>). Data collections confirmed the displacive first-order triclinic $\overline{1}$-12/c phase transition at $P ~ 4.3$ GPa found in a previous high-P investigation and defined the first-order monoclinic-monoclinic transformation at $P ~ 7.3$ GPa as an 12/c-P2<sub>1</sub>/c symmetry change. The structural modifications induced by the increase of pressure inside the stability fields of $\overline{1}$ and 12/c configurations as well as the structural behavior of the two phase transitions were detailed. The $\overline{1}$-12/c transition is similar to the displacive ferroelastic $\overline{1}$-12/c phase transition observed for the same composition with increasing temperature and is related to the increase of the M-site coordination number, with the consequent regularization of Ca/Sr polyhedra and framework. Variations of the T-O-T bond angles are observed, whereas the O-T-O angles do not change significantly.

The 12/c-P2<sub>1</sub>/c transition involves a significant modification of the M-polyhedra. In the M(0)-polyhedron, the two O<sub>2</sub> atoms, that were not coordinated in $\overline{1}$ and 12/c space groups, are now bonded more strongly than either O<sub>0</sub> or O<sub>1</sub> atoms [the M(0)-O<sub>2</sub>(0i) and M(0)-O<sub>2</sub>(zi) distances are 2.54 and 2.57 Å, respectively]. In the M(i)-polyhedron, it is the second O(20) oxygen that becomes coordinated and, at the same time, one of the bonds to O<sub>0</sub> atoms is broken. Moreover, a significant deformation of the framework is obtained due to the decrease of the symmetry from the loss of the two-fold axis and of half of the centers of symmetry. The transition induces, besides a significant distortion in the T-O-T bond angles, a deformation of the internal O-T-O angles within the tetrahedra. The T<sub>2</sub>(00) tetrahedron, with the O(20)-T<sub>2</sub>(00)-O<sub>C</sub>(0i) angle of 91° and the O<sub>C</sub>(0i)-T<sub>2</sub>(00)-O<sub>D</sub>(0i) angle of 140°, is the most deformed.

Keywords: Crystal structure, high-pressure studies, phase transition, XRD data

INTRODUCTION

The feldspar structure has been well defined by crystallographic studies performed on natural and synthetic end-members and different solid solutions at both ambient conditions and at high temperatures and pressures (see the excellent reviews of Ribbe 1994 on crystal structure and of Angel 1994 and Ross 2000 on the high-pressure behaviors).

Structural investigations performed on alkali feldspars using high-pressure in situ single-crystal X-ray diffraction include those of Allan and Angel (1997) (microcline to $P = 7$ GPa), Downs et al. (1994), and Benusa et al. (2005) (compression of low albite to 4 GPa and 9.4 GPa, respectively). The structure of reedmergnerite has been refined by Downs et al. (1999) to 4.7 GPa. No phase transitions were observed in these feldspars with increasing pressure (the $C2/m$-C$\overline{1}$ transition observed in sanidine at $P = 1.8$ GPa by Hazen 1976 has not been confirmed). On the contrary, Angel et al. (1988) observed a reversible first-order PT-12/c phase transition between 2.6 and 3 GPa in anorthite. Angel (1988) determined the structural configurations of the PT and 12/c phases by means of in situ structural investigations at high-pressure.

Recently, Nestola et al. (2004) observed pressure induced phase transitions in a feldspar of composition Ca<sub>0.2</sub>Sr<sub>0.8</sub>Al<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>, which lies on the solid solution between triclinic PT anorthite (An, CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>) and monoclinic 12/c Sr-feldspar (SrF, SrAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>). Along this join at ambient conditions the symmetry changes from 12/c to PT at a composition of ~An<sub>20</sub>SrF<sub>80</sub>. Moreover, feldspars with compositions between An<sub>20</sub>SrF<sub>80</sub> and An<sub>20</sub>SrF<sub>80</sub> undergo the analogous 12/c-P2<sub>1</sub>/c transition with increasing temperature. The 12/c-P2<sub>1</sub>/c phase transition (Bruno and Gazzoni 1968; Nager 1969; Nager et al. 1969; Tribaudino et al. 1993)