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The high-pressure structural configurations of $Ca_{0.2}Sr_{0.8}Al_2Si_2O_8$ feldspar: The $I\bar{1}$-$I2/c$ and $I2/c$-$P2_1/c$ 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 $Ca_{0.2}Sr_{0.8}Al_2Si_2O_8$ feldspar ($An_{20}SrF_{80}$). Data collections confirmed the displacive first-order triclinic $I\bar{1}$-monoclinic $I2/c$ 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 $I2/c$-$P2_1/c$ symmetry change. The structural modifications induced by the increase of pressure inside the stability fields of $I\bar{1}$ and $I2/c$ configurations as well as the structural behavior of the two phase transitions were detailed. The $I\bar{1}$-$I2/c$ transition is similar to the displacive ferroelastic $I\bar{1}$-$I2/c$ 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 $I2/c$-$P2_1/c$ transition involves a significant modification of the M-polyhedra. In the M(0)-polyhedron, the two O_C atoms, that were not coordinated in $I\bar{1}$ and $I2/c$ space groups, are now bonded more strongly than either O_B or O_D atoms [the M(0)-O_C(0i) and M(0)-O_C(zi) distances are 2.54 and 2.57 Å, respectively], whereas in the M(i)-polyhedron, it is the second OA(20) oxygen that becomes coordinated and, at the same time, one of the bonds to O_D 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_2(00) tetrahedron, with the OA(20)-T_2(00)-O_C(0i) angle of 91° and the O_C(0i)-T_2(00)-O_D(0i) angle of 140°, is the most deformed.

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