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Single-crystal in situ high-temperature structural investigation of the $I\bar{1}$– $I2/c$ phase transition in $Ca_{0.2}Sr_{0.8}Al_2Si_2O_8$ feldspar

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ABSTRACT

Structural modifications induced by the $I\bar{1}$-$I2/c$ displacive transition in $Ca_{0.2}Sr_{0.8}Al_2Si_2O_8$ feldspar ($An_{20}SrF_{80}$) have been investigated in situ by single-crystal X-ray diffraction at 20, 200, 400, 500, and 620 °C. Crystals were synthesized from the melt, cooled slowly to 1300 °C, and then quenched in air. At room temperature (a = 8.361, b = 12.973, c = 14.259 Å, α = 90.79, β = 115.55, γ = 90.62°, V = 1394.9 Å^3; space group: $I\bar{1}$; Q_{od} = 0.88), the polyhedra of the non-tetrahedral cation have different configurations at the Ca/Sr(0) and Ca/Sr(z) sites. In monoclinic Sr feldspar, the Sr-O_B and Sr-O_D distances are regular, but in triclinic $An_{20}SrF_{80}$ feldspar the O_B(m0) atom in the Ca/Sr(0)-polyhedron and the O_D(mz) atom in the Ca/Sr(z)-polyhedron are displaced. The topochemical symmetry of the framework is essentially monoclinic and the average dimensions of the pseudo-symmetrical tetrahedra do not change within the error limits. With increasing temperature, the distances between the Ca/Sr cations and the pseudo-related O atom pairs converge on the values adopted at the $I\bar{1}$-$I2/c$ transition. At the transition point, the M-polyhedron assumes a regular coordination, similar to that observed in monoclinic Sr feldspar at room temperature. The results obtained indicate T_{tr} = 520 ± 10 °C, in agreement with the transition temperature obtained from the changes of cell dimensions. The variation of $\cos^2\alpha^*$ with temperature is consistent with the solution to Landau 2-4-6 potential with T_c = 506 ± 7 °C.