

Si-Al order and the $I\bar{1}-I2/c$ structural phase transition in synthetic $\text{CaAl}_2\text{Si}_2\text{O}_8$ - $\text{SrAl}_2\text{Si}_2\text{O}_8$ feldspar: A ^{29}Si MAS-NMR spectroscopic study

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ABSTRACT

We present ^{29}Si MAS-NMR spectroscopic data for a series of synthetic feldspar samples along the join $\text{CaAl}_2\text{Si}_2\text{O}_8$ - $\text{SrAl}_2\text{Si}_2\text{O}_8$, from which the composition dependence and coupling of order parameters describing Si-Al order and the triclinic-monoclinic displacive transition were determined. Spectra of $\text{SrAl}_2\text{Si}_2\text{O}_8$ contain narrow peaks for the two crystallographic Si sites, plus additional peaks for Si having three and two Al nearest neighbors, indicating the presence of approximately 0.14 Al-O-Al linkages per formula unit and a value of $\sigma = 0.93$ for the short-range order parameter. For the triclinic feldspar samples, short-range Si-Al order increases continuously with Sr content from $\sigma = 0.89(3)$ for $\text{CaAl}_2\text{Si}_2\text{O}_8$ to $0.97(1)$ for $\text{Sr}_{0.80}\text{Ca}_{0.20}\text{Al}_2\text{Si}_2\text{O}_8$ but then decreases discontinuously to $0.93(2)$ for the monoclinic samples, $\text{Sr}_{0.85}\text{Ca}_{0.15}\text{Al}_2\text{Si}_2\text{O}_8$ to $\text{SrAl}_2\text{Si}_2\text{O}_8$. The variation of peak positions with composition is consistent with a structural phase transition near $\text{Sr}_{0.85}\text{Ca}_{0.15}\text{Al}_2\text{Si}_2\text{O}_8$ from $I\bar{1}$ to $I2/c$. The order parameter for this displacive transition is reflected by the chemical shift of the T1mz crystallographic site, and its composition dependence gives an order-parameter critical exponent of $\beta = 0.49(2)$, indicating classical second-order behavior.