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Lattice simulation studies of the ferroelastic phase transitions in $(Na,K)AlSi_3O_8$ and $(Sr,Ca)Al_2Si_2O_8$ feldspar solid solutions

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ABSTRACT

Lattice-energy minimization calculations have been performed on the feldspar systems $(Ca,Sr)Al_2Si_2O_8$ and disordered $(Na,K)AlSi_3O_8$ as functions of composition to simulate the ferroelastic phase transitions $I2/c$–$I\bar{1}$ and $C2/m$–$C\bar{1}$, respectively. In both cases the phase transition occurs as a function of composition and is driven by the vanishing of the quantity $C_{44}C_{66} - C_{46}^2$, without any of the individual elastic constants being strongly dependent on composition and without softening of an optic mode. In both cases, the strains ϵ_4 and ϵ_6 are proportional to each other for small values of strain, but nonlinear coupling becomes dominant when $|\epsilon_4|$ becomes larger than about 0.02. The results are consistent with experimental data and explain the nature of coupling of the displacive transition to Al-Si ordering in Al:Si 2:2 feldspars.