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Molecular dynamics simulation of Al/Si-ordered plagioclase feldspar

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ABSTRACT

Molecular dynamics (MD) simulations of the thermodynamic properties of Al/Si-ordered plagioclase were performed for two different crystallographic configurations: a solid solution structure and a lamellar structure. MD-simulated plagioclase feldspar solid solution has three space groups—$C\bar{1}$, $I\bar{1}$, and $P\bar{1}$—at 300 K, and two space groups—$C\bar{1}$ and $I\bar{1}$—at higher temperatures. In addition, the MD-simulated, composition-dependent $I\bar{1}$-$C\bar{1}$ and $P\bar{1}$-$I\bar{1}$ phase transitions are non-first order. However, the temperature-dependent $I\bar{1}$-$C\bar{1}$ phase transition is not observed for any plagioclase composition. The calculated excess enthalpy and excess Gibbs free energy of the MD-simulated solid solution structure are convex upward, and for a given plagioclase composition the excess Gibbs free energy of the MD-simulated lamellar structure is smaller than that of the MD-simulated solid solution structure. These results indicate that a lamellar structure (created by phase separation) consisting of fully ordered albite and anorthite is more stable than the solid solution structure, which consists of randomly distributed clusters of both phases. Therefore, when plagioclase feldspar is heated for a long period of time at a low temperature, phase separation between pure albite and pure anorthite can be expected if equilibrium is achieved.