Molecular dynamics simulation of plagioclase feldspar

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Molecular dynamics (MD) simulations for the thermodynamic properties of ordered plagioclase feldspar were carried out by using two different types of structure with cluster-random structure and the lamella structure. The excess enthalpy and the free energy of MD-simulated cluster-random structure were concaved upward and the excess enthalpy of MD-simulated lamella structure was smaller than that of MD-simulated cluster-random structure with same composition. These results show the possibility of the phase separation between pure albite and pure anorthite in ideal plagioclase feldspar such as that the annealing time is infinite at lower temperature.