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The dickite and nacrite minerals behavior under high-pressure

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Abstract

We studied the behavior of dickite and nacrite minerals under pressures up to 14 GPa by means of the molecular dynamics simulations based on energy minimization technique. We found probable phases transitions in the structures of dickite and nacrite minerals and focused on analysis of their respective structural properties. Phase transitions of minerals are strongly related to structural instability and can therefore induce changes in the elastic behaviour. The behaviour of elastic properties can give an indication of the high-pressure phase transition. Phase transitions in dickite and nactire structures were found around 13.3 GPa and 9.7 GPa, respectively. The lattice parameters of nacrite and dickite show an abrupt change along the curve of the structural and elastic properties, which may indicate a modification of their structure.

Keywords:

Phase transition dickite nacrite molecular dynamics simulation high-pressure