Molecular dynamics simulation of phase transition between high-temperature and high-pressure clinoenstatite

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Phase transformation between high-temperature (HT-CEn) and high-pressure clinoenstatites (HP-CEn) was studied using molecular dynamics (MD) simulations. Starting from HT-CEn, the MD simulations of isothermal compression were carried out at different temperatures. At 2800 and 2500 K, HT-CEn directly transformated into HP-CEn at high pressure and the discontinuous change of the MD-simulated cell volume between HT-CEn and HP-CEn showing an isosymmetric or first-order transition was observed. A phase relation of CEn's is also proposed, although clinoenstatite is metastable with respect to orthoenstatites at low pressure.