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Isosymmetric structural phase transition of orthoenstatite: Molecular dynamics simulation

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Abstract

An isosymmetric phase transition from orthoenstatite to a new high-temperature orthorhombic phase of enstatite was observed at about 1230 K in molecular dynamics (MD) simulations for the Mg end-member composition, $Mg_2Si_2O_6$. This new phase has the same space group as orthoenstatite, *Pbca*. The discontinuous changes of the cell volume and cell parameters during the transition indicate a first-order transition. The transition is characterized by the switching of bonds between Mg atoms at the M2 sites and the coordinated O3 atoms. This new phase corresponds to the high-temperature state of enstatite observed in the in situ high-temperature X-ray studies and probably to orthopyroxene appearing in the phase diagram of the quadrilateral pyroxenes, indicating the possibility of its existence as a stable phase at high temperature.