American Mineralogist, Volume 94, pages 950–956, 2009

Phase behavior of protoenstatite at high pressure studied by atomistic simulations

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Abstract

Structural phase transformations of $MgSiO_3$ protoenstatite at high pressures are studied by atomic scale simulation techniques. Molecular-dynamics simulations and electronic-structure calculations reveal two metastable polymorphs with space groups $P2_1cn$ and $Pbcn$, respectively. They are related to protoenstatite by displacive transition mechanisms via subsequent change of the silicate chain rotations from O- to S-type. Metadynamics simulations in combination with molecular dynamics reveal possible mechanisms for the martensitic transition from protoenstatite to high-pressure clinoenstatite. Two different shear mechanisms in the (100) plane are activated during the transition. The first consists of four partial displacements in (100)[001] and (100)[010], whereas in a second step only a single shear in (100)[001] is observed.

Keywords: Molecular dynamics, metadynamics, phase transition, enstatite, $MgSiO_3$, protopyroxene, clinopyroxene