

Molecular dynamics simulation of orthoenstatite under high temperature and pressure

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Enstatite, Mg end member of pyroxene, has several polymorphs, ortho enstatite (Oen), proto enstatite (Pen), and clino enstatite (Cen). Cen is divided into three phases, low temperature clino enstatite (LT-Cen), high temperature clino enstatite (HT-Cen), and high pressure clino enstatite (HP-Cen). Recently isosymmetric structural phase transition of Oen was experimentally confirmed by Ohi et al. (2008). Phase transition between low temperature (LT-Oen) and high temperature Oen (HT-Oen) was confirmed with in-situ X-ray method at 1atm., but pressure dependence of this phase transition is less well understood yet. On the other hand, at higher pressure and temperature conditions, the Oen phase undergoes a reconstructive transformation to the HP-Cen phase. Recently Kung et al. (2004) observed a substantial softening of the bulk modulus above 10 GPa and before the intended transition from OEn to HP-CEn. Jahn (2008) suggested two possible high pressure polymorphs of Oen, one with P21ca and the other with Pbc symmetry by using Molecular dynamics (MD) simulations and first-principles electronic structure calculations. In this study, The behavior of orthoenstatite at high temperature and pressure was studied by using MD simulation technique 1; to determine dP/dT of the phase transition from LT-Oen to HT-Oen and 2; to investigate possible existence of HP-Oen phase.

The MD simulation was carried out on the basis of an interatomic potential model which is taken to be the sum of Coulomb, van der Waals attraction, short range repulsion, and Morse potential terms. The potential parameters used in this study were determined empirically by Miyake et al. (1998). The program MXDTRICL (Kawamura,2005) was used for MD simulation, with triclinic system in which angles of alpha, beta, and gamma do not have constant value, 90 degree, but are variable. Starting from the structure of orthoenstatite determined by the X-ray method as the initial state, the annealing MD calculations were carried out.

1;As results, first order phase transition from LT-Oen to HT-Oen was observed around 1200K, 1atm. The phase transition temperature from LT-Oen to HT-Oen increases with increasing pressure. And at 6GPa, continuous phase transition was observed.

2;Under higher pressure, over 15GPa at 1500K, discontinuous volume change to new phase was observed and beta value was not 90 degree. These results showed that this phase transition is first order, and new high pressure phase is monoclinic phase. The a-axis of this monoclinic phase is two times longer than LT-Cen and HP-Cen. No Oen phases such as P21ca or Pbc were found under high pressure condition in this study.