American Mineralogist, Volume 83, pages 937–941, 1998

Molecular dynamics simulation of phase transitions and melting in $MgSiO_3$ with the perovskite structure

S.L. Chaplot,* N. Choudhury, and K.R. Rao

Solid State Physics Division, Bhabha Atomic Research Center, Trombay, Mumbai 400085, India

Abstract

The high pressure phase transitions and melting of the mantle mineral $MgSiO_3$ with the perovskite structure were investigated using molecular dynamics (MD) simulations of a large system of atoms on a parallel computer. The simulations reveal an orthorhombic to cubic transition accompanied by a sharp increase in diffusion of the O atoms. The phase transition and melting temperature depend sensitively on the level of defects in the solid. At pressures of the Earth's lower mantle, the transition is found to occur at temperatures substantially higher than the mantle temperatures. Therefore, any seismic discontinuity in the lower mantle may not be related to a phase transition of the perovskite structure, but instead may be due to chemical changes at that depth, in contrast to currently accepted mineralogical models assuming chemical homogeneity of the lower mantle.