American Mineralogist, Volume 85, pages 317–320, 2000

Ab initio structure of $MgSiO_3$ ilmenite at high pressure

B.B. KARKI, W. DUAN, C.R.S. DA SILVA, AND R.M. WENTZCOVITCH*

Department of Chemical Engineering and Materials Science, Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, Minnesota 55455, U.S.A.

ABSTRACT

The structural properties of $MgSiO_3$-ilmenite at high pressures are determined using Ab initio variable cell-shape molecular dynamics. Our athermal results at zero pressure are in excellent agreement with single-crystal measurements. The predicted lattice constants compare favorably with powder X-ray diffraction data. The internal parameters are shown to vary only slightly with pressure. The *c* axis is considerably more compressible than the *a* axis and our results suggest that this anisotropic behavior arises in the relatively larger compressibility of MgO_6 with respect to SiO_6 octahedra. Both octahedral types remain highly distorted with the degree of distortion decreasing (more rapidly in MgO_6) under compression. By comparing free energies, it is shown that $MgSiO_3$ should transform from the ilmenite to the perovskite structure at 30 GPa (for static lattice). At the transition, the density and elastic moduli increase substantially.