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Reinvestigation of the $MgSiO_3$ perovskite structure at high pressure

MASAHIKO SUGAHARA,[1] AKIRA YOSHIASA,[1,*] YUTAKA KOMATSU,[2] TAKAMITSU YAMANAKA,[2] NATHALIE BOLFAN-CASANOVA,[3] AKIHIKO NAKATSUKA,[4] SATOSHI SASAKI,[5] AND MASAHIKO TANAKA[6]

[1]Faculty of Science, Kumamoto University, Kumamoto 860-0909, Japan
[2]Graduate School of Science, Osaka University, Osaka 560-0043, Japan
[3]Laboratoire Magmas et Volcans, University of Blaise, Pascal CNRS, France
[4]Faculty of Engineering, Yamaguchi University, Ube 75-8611, Japan
[5]Tokyo Institute of Technology, Nagatsuta 4259, Yokohama 226-8502, Japan
[6]Photon Factory, KEK, Tsukuba, Ibaraki 305-0801, Japan

ABSTRACT

High-pressure single-crystal X-ray diffraction experiments of $MgSiO_3$ perovskite have been carried out up to 15 GPa in a diamond-anvil cell using synchrotron radiation. Precise crystal structural parameters, including the anisotropic displacement parameters of every atom in $MgSiO_3$, are determined under high pressure. In the pressure range up to 15 GPa, the most important responses of the structure are the compressions of SiO_6 and MgO_8 polyhedra and an increase in tilting of SiO_6 octahedra represented by the decrease in angles between octahedra (both Si-O2-Si angle in the *a-b* plane and Si-O1-Si angle in the *b-c* plane decrease). The degree of the change in both angles in the *a-b* and *b-c* planes is the same. The amplitude of mean square displacement for the Mg atom has the largest value in the structures and its thermal vibration is significantly anisotropic at ambient pressure. Under high pressure, all atoms in the structure have obvious anisotropy of thermal vibration and the largest amplitudes of thermal vibration for Mg, Si, and O2 atoms are directed toward vacant space in the structure. Anisotropy of the structure increases with pressure.

Keywords: Crystal structure, high-pressure study, $MgSiO_3$ perovskite, pressure responses, thermal vibration