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The crystal structures of natural norbergite at 4.7 and 6.3 GPa conditions

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Introduction

Norbergite ($Mg_2SiO_4 \cdot Mg(OH,F)_2$), which is a hydrous magnesium silicate mineral, is known as one of the humite minerals described as $nMg_2SiO_4 \cdot Mg(OH,F)_2$ (n=1-4). This mineral has the similar structure to forsterite (Mg_2SiO_4), which is recognized as the most important mineral in the mantle of the earth, and is given much attention as the carriers and reservoirs of water in the subduction zone. The stability of humite minerals has been studied some researchers (*ex.* [1], [2]). Forsterite and the humite minerals constitute the polysomatic series.

We collected the X-ray reflection intensity data sets of a natural norbergite at ambient, 4.7 and 6.3 GPa in order to investigate its crystal structure. In this report, we described the crystal structures at 4.7 and 6.3 GPa.

Experimental Procedure

The sample used for this study is from Sterling Hill Mine, New Jersey, U.S.A. A single crystal of norbergite (60×50×40 μm^3 in size) was mounted in a modified Merrille-Bassett type diamond anvil cell with a small piece of a ruby crystal, which used for the pressure calibration. The 4:1 fluid mixture of methanol and ethanol was used for the pressure medium and a SUS301 stainless plate used for a gasket. Pressure was determined by the ruby fluorescence method [3]. The wavelength of X-ray was calibrated by the unit cell volume of the ruby standard crystal at ambient temperature (λ = 0.7002 Å). The X-ray diffraction intensities were measured using an automated four-circle X-ray diffractometer installed at the beam line BL-10A, Photon Factory, High Energy Accelerator Research Organization. The X-ray reflection intensity data sets at 4.7 and 6.3 GPa were collected up to $\sin\theta/\lambda$ < 0.82 Å^{-1} (maximum 2θ is 70.0°). The 3/8 of a reciprocal sphere was measured. A total of 1346 (for 4.7 GPa) and 1259 (for 6.3 GPa) reflections were obtained. After background and Lorentz corrections were applied to all measured reflections, the symmetrically equivalent reflections were averaged by the Laue symmetry of *mmm*. The number of 441 and 399 reflections ($Fo > 2.0\sigma(Fo)$) were used for the structure refinement, respectively. The previous model at ambient conditions [4] was used for the initial parameters of the norbergite structure (Space group *Pbnm* (#62)). The sigma weights were applied to the all obtained reflection data. Final agreement factors were R = 5.7 and 6.7 % and R_w = 5.4 and 5.9 %, respectively. All calculations were performed using the teXsan crystallographic software. The unit cell parameters of norbergite were reported by our previous report [5].

Results

Polyhedral bulk moduli of each polyhedron were calculated using the Birch-Murnaghan equation of state with a pressure derivative $K' = 4$. K_{M2} = 106 (5) GPa, K_{M3} = 113(2) GPa and K_{Tet} = 293(15) GPa. In norbergite structure, octahedral bulk moduli were smaller than the corresponded those of humite minerals and forsterite (K_M = 130 - 150 GPa, [5], [6]). In contrast, K_{Tet} of tetrahedron is smaller than (K_{Tet} = 190 GPa, [6]) that of forsterite, which has the same environment for tetrahedron (Fig. 1). The octahedral-tetrahedral shared edges (O2-O3 and O3-O3; β_{O2-O3} and β_{O3-O3} were 1.25(19) and 0.97(19) × 10^{-3}GPa^{-1}, respectively) were stiffer than the other O-O distances (averaged the other β_{O-O} was 2.89 × 10^{-3}GPa^{-1}).
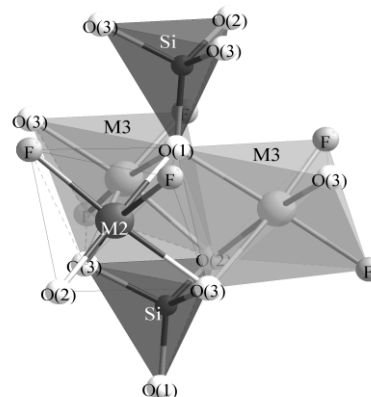
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