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The effects of pressure on the crystal structure of humite, $Mg_7Si_3O_{12}(OH, F)_2$

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Introduction

Humite, which is a hydrous magnesium silicate mineral, is known as one of the humite minerals described as $n\mathrm{Mg_2SiO_4{\cdot}Mg(OH, F)_2}$ (n=1-4). Forsterite, Mg_2SiO_4, is the most important mineral in the minerals constituted of the Earth′s mantle. Forsterite and the humte minerals constituted the polysomatic series. The humite minerals are important in the view of the carriers and reservoirs of water in the Earth′s deep interior, because these minerals are stable under high-pressure and high-temperature mantle conditions[1].

We performed a high-pressure single crystal X-ray diffraction study on humite at 5.1 and 6.3 GPa in order to investigate the effects of pressure on the crystal structure of this mineral. In this paper, we reported the crystal structure of humite at 5.1 GPa and some physical properties such as the isothermal bulk modulus and the axial linear compressibility of humite, which calculated from this result and our previous data[2].

Experimental Procedure

The sample used for this study is from Tilley Foster Mine, Brewster, New York, U.S.A.. A single crystal of humite (50×40×30 μm 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 synchrotron radiation (λ=0.6955 Å for 5.1 GPa and λ=0.6946 Å for 6.3 GPa) was calibrated by the unit cell volume of the ruby standard crystal at ambient temperature. The X-ray diffraction data 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 unit cell parameters of humite at 5.1 GPa and 6.3 GPa were determined from 25 centered reflections in the 2θ range between 14.9° and 27.5°. The X-ray reflection intensity data at 5.1 GPa were collected up to $\sin\theta/\lambda < 0.70$ Å^{-1} (maximum 2θ is 65.0°). The 3/8 of a reciprocal sphere was measured. A total of 2714 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*. 452 reflections ($Io > 2.0\sigma(Io)$) were used for the structure refinement at 5.1 GPa. Our previous data at 2.7 GPa[2] were used for the initial parameters of the humite structure (Space group *Pbnm*). The Cruickshank weights were applied to the all obtained reflection data. Final agreement factors were R=5.6% and Rw=9.2%. All calculations were performed using the teXsan crystallographic software[4].

Results

The unit cell parameters of humite at 5.1 and 6.3 GPa were determined as a=4.698(4)Å, b=10.106(6)Å, c=20.599(3)Å for 5.1 GPa data set and a=4.687(4)Å, b=10.080(7)Å, c=20.548(3)Å for 6.3 GPa. The linear axial compressibilities of humite at each pressure were calculated using these results and our previous data[2], yielding to β_a=1.70(6), β_b=2.92(8) and β_c=2.45(5) ($\times 10^{-3}$ /GPa). The $\beta_b > \beta_c > \beta_a$ trend was the same as those of the other humite minerals. In similarly, the isothermal bulk modulus of humite was calculated as K=130(2) GPa assuming K′=4. This result is consistent with the simple positive correlation[5] between K and density (ρ) for the minerals on the brucite-forsterite line. The final atomic coordinates are given in Table 1.

Table 1. Final atomic coordinates of humite at 5.1 GPa

Site	x	y	z	B_{iso}
M1	0.0015(6)	0.3781(4)	0.1767(1)	0.67(4)
M2	0.5119(8)	0.1533(5)	0.25	1.18(5)
M3	0.0094(6)	0.0989(4)	0.1091(1)	0.70(5)
M4	0.4933(6)	0.8675(5)	0.0278(1)	0.49(5)
Si1	0.0737(8)	0.9702(5)	0.25	0.53(5)
Si2	0.5755(5)	0.2825(4)	0.1060(1)	0.44(4)
O11	0.7345(20)	0.9652(16)	0.25	1.03(3)
O12	0.2782(18)	0.3226(11)	0.25	0.54(4)
O13	0.2256(13)	0.0400(11)	0.1876(3)	0.61(5)
O21	0.2344(12)	0.2810(11)	0.1050(3)	0.63(5)
O22	0.7794(13)	0.9297(8)	0.1041(3)	0.58(5)
O23	0.7228(12)	0.2133(10)	0.1692(3)	0.57(5)
O24	0.7254(13)	0.2077(8)	0.0445(3)	0.57(5)
OH	0.2579(12)	0.0316(8)	0.0357(3)	0.85(5)

References

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