American Mineralogist, Volume 84, pages 199–202, 1999

LETTERS

Structure refinement of a birefringent Cr-bearing majorite $Mg_3(Mg_{0.34}Si_{0.34}Al_{0.18}Cr_{0.14})_2Si_3O_{12}$

AKIHIKO NAKATSUKA,[1] AKIRA YOSHIASA,[2] TAKAMITSU YAMANAKA,[2] AND EIJI ITO[3]

[1]Department of Advanced Materials Science and Engineering, Faculty of Engineering, Yamaguchi University, Ube, Yamaguchi 755-8611, Japan
[2]Department of Earth and Space Science, Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan
[3]Institute for Study of the Earth's Interior, Okayama University, Misasa, Tottori 682-0193, Japan

ABSTRACT

A single crystal of a birefringent Cr-bearing majorite, $Mg_3(Mg_{0.34}Si_{0.34}Al_{0.18}Cr_{0.14})_2Si_3O_{12}$, was synthesized at 20 GPa and 2000 °C using "6–8" type uniaxial split-sphere apparatus. This garnet is tetragonal with the unit-cell parameters $a \approx c$ and deviates slightly from cubic symmetry. The structure refinements using single-crystal X-ray diffraction intensity data were carried out by assuming three space groups (one cubic and two tetragonal) to determine the most probable symmetry. The most probable space group is $I4_1/a$ (tetragonal). The Cr ions show a disordered distribution between the two nonequivalent octahedral sites in the $I4_1/a$ structure.

INTRODUCTION

The seismic discontinuities in the Earth's mantle are controlled by changes in the physical properties of the constituent mineral phases. Therefore, the investigation of the symmetry of mantle minerals is important because the physical properties are very sensitive to the crystal structure. The majorite solid-solution in the system $Mg_3Al_2Si_3O_{12}$-$MgSiO_3$ having the garnet structure is considered to be a major constituent of the transition zone in the Earth's mantle between the 400 and 670 km seismic discontinuities (e.g., Ringwood 1967; Liu 1977; Akaogi and Akimoto 1977; Ito and Takahashi 1987). It has been reported that the symmetry of the majorite solid-solution with 20–100 mol% $Mg_3Al_2Si_3O_{12}$ component is cubic (space group $Ia\bar{3}d$), whereas that of garnet having a $MgSiO_3$ composition is tetragonal (space group $I4_1/a$) (e.g., Kato and Kumazawa 1985; Sawamoto 1987; Angel et al. 1989; Parise et al. 1996; Heinemann et al. 1997). The cubic phase ($Ia\bar{3}d$) has one unique dodecahedral (X), octahedral (Y), tetrahedral (Z), and oxygen (O) site, whereas the tetragonal phase ($I4_1/a$) has two nonequivalent dodecahedral (X1 and X2), two octahedral (Y1 and Y2), three tetrahedral (Z1–Z3), and six oxygen (O1–O6) sites. The end-member $MgSiO_3$ garnet exhibits ordering of Mg and Si between Y1- and Y2-sites in the $I4_1/a$ structure (Angel et al. 1989).

The upper mantle contains about 0.4 wt% Cr_2O_3 (Ringwood 1979) and most of the Cr ions in transition zone in the Earth's mantle are expected from high-pressure experiments by Irifune (1994) to be distributed to the high-pressure garnet phase, i.e., the majorite solid-solution. Hence, the behavior of Cr ions in the majorite solid-solution in the Earth's mantle cannot be neglected. In the present study, we examine the symmetry of Cr-bearing majorite and the distribution of Cr ions between atomic sites in the crystal structure using the single-crystal X-ray diffraction method.

EXPERIMENTAL DETAILS

Material

A single crystal of Cr-bearing majorite, $Mg_3(Mg_{0.34}Si_{0.34}Al_{0.18}Cr_{0.14})_2Si_3O_{12}$, was synthesized under high pressure and high temperature (20 GPa and 2000 °C) using a 1000 ton "6–8" type uniaxial split-sphere apparatus (USSA-1000) installed at the ISEI of Okayama University. Special grade reagents (99.99%) of MgO, α-Al_2O_3, SiO_2, and Cr_2O_3 were used as starting materials. These oxides were mixed together in a stoichiometric molar ratio. A flux of PbO (15 mol%) was mixed with the starting materials. The anvil assembly of tungsten carbide cubes with a truncated edge length of 5 mm was compressed with the aid of USSA-1000. A 10 mm regular octahedron of a sintered MgO containing 5% Cr_2O_3 was used as pressure medium. The powder mixtures were put into a cylindrical rhenium heater embedded in the MgO octahedron. Because MgO has a high thermal conductivity, a $LaCrO_3$ sleeve was inserted outside of the rhenium heater. The sample temperature was monitored by a W25%Re-W3%Re thermocouple with 0.05 mm in diameter. The junction of the thermocouple was put at the midpoint of the outer surface of the cylindrical rhenium heater. No correction was made for the pressure effect on emf. After being kept at 20 GPa and 2000 °C for an hour, the product was quenched by shutting off the electric power supply. The pressure was released slowly and the product was recovered under ambient conditions. Composition of the single crystal was determined using a JEOL JCMA-733II electron microprobe analyzer (EPMA). No contamination of Pb into the single crystal was detected from

---

*E-mail: tuka@po.cc.yamaguchi-u.ac.jp

0003-004X/99/0102–0199$05.00