Crystallography

10A/2006G254

Crystal Structure of High Pressure phase of $MgAl_2O_4$ synthesized at conditions of 2200 K and 41.8 GPa

Yasuhiro KUDOH*[1], Takahiro KURIBAYASHI[1], Yuichiro SUEDA[2], Tesuo IRIFUNE[2] and Satoshi SASAKI[3]
[1]Institute of Mineralogy, Petrology, and Economic Geology, Faculty of Science, Tohoku University, Sendai 980-8578, Japan
[2]Geodynamics Research Center, Ehime university, Matsuyama 790-8577, Japan
[3]Materials and Structures Laboratory, Tokyo Institute of Technology Nagatuda Yokohama 226-8503, Japan

The specimen used in this study was a single crystal of high pressure phase of $MgAl_2O_4$ synthesized using a multi-anvil apparatus at conditions of 2200 K and 41.8 GPa [1] and quenched to ambient condition by Sueda et al. (2004). EDS analysis showed that the specimen has a chemical composition of ideal formula $MgAl_2O_4$ within the limit of erperimental error. Sets of X-ray diffraction intensities were measured with a single crystal of 47x47x24 μm using synchrotron radiation at the beam line BL-10A, Photon Factory, High Energy Accelerator Reasearch Organization, Tukuba, Japan. The wave length, λ=0.7009 Å was calibrated by the unit cell constants of a ruby standard crystal (*a*=4.76099(6) Å, c=12.99625(35) Å). The crystallographic data obtained are: orthorhombic, *a*=2.781(3) Å, *b*=9.183(3) Å, *c*=9.383(3) Å, *V*=239.6(3) Å^3. The systematic abscences and *N*(*Z*) test for a center of symmetry indicated the centrosymmetric space group *Cmcm* (No.63). From the total of 2043 reflections measured in the sphere of $\sin\theta/\lambda = 1.00$ Å^{-1}, 1264 symmetry-independent reflections were obtained by averaging the symmetry equivalent intensities in Laue group *mmm* (R_{int} = 11%).

The crystal structure is isostructural with $CaTi_2O_4$ (CT-tyoe) and refined to an *R*=8.7 % (*R*w=8.3%) with anisotropic temperature factors. The calculated density value 3.94 g/cm^3 is 10% larger than 3.578 g/cm^3 value of spinel (SP-type), $MgAl_2O_4$ [2] which is the stable phase at ambient condition. The Mg atom is surrouded by 6 oxygen atoms with the average Mg-O distance being 2.142(4) Å and another 2 oxygen atoms at 2.558(1) Å with the average Mg-O distance being 2.246(4) Å for 8 fold coordination. The Al atom is surrouded by 6 oxygen atoms with the average Al-O distance being 1.921(3) Å which is comparable to the 1.926 Å value of spinel [2]. Fig. 1 is the comparison of MgO_4 group in SP-type and MgO_6 group in CT-type viewed along the direction perpendicular to the basal trangles of MgO_4 tetrahedra and MgO_6 octahedra, showing a syntaxial relation between two structures.

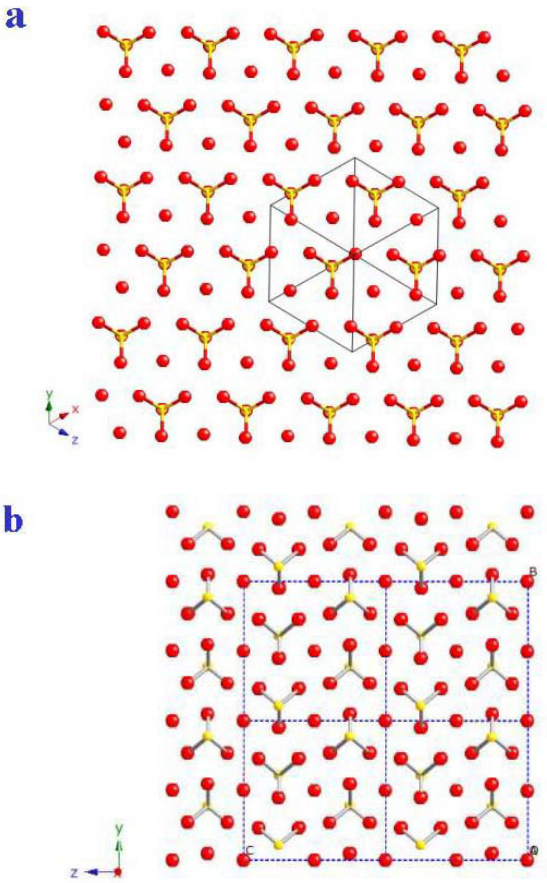

Fig. 1. Comparison of **a** MgO_4 group in SP-type $MgAl_2O_4$ and **b** MgO_6 group in CT-type $MgAl_2O_4$.

References

[1] Y. Sueda, T. Irifune, T. Inoue, Y. Higo, T. Kunimoto, H. Namura and K. Funakoshi: Mineralogical Society of Japan 2004 Annual Meeting, Abstr., p.25 (2004)
[2] P. Fischer: Z. Kristallogr., 124, 275-302 (1967)

*ykudoh@m.tains.tohoku.ac.j