

Single-crystal X-ray diffraction study on new high-pressure forms of Al_2SiO_5 Takahiro KURIBAYASHI^{1*} and Toshiro NAGASE²¹ Department of Earth Science, Graduate School of Science,
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1 Introduction

The system of Al_2O_3 - SiO_2 is important for the fields of Earth Science and Material Science for Ceramics. Especially, Al_2SiO_5 minerals in this system such as kyanite, andalusite and sillimanite are valuable for estimation of pressure and temperature conditions in metamorphic rocks.

In Earth Science field, recently, Zhou et al. (2018) [1] have reported that new high-pressure forms of Al_2SiO_5 were synthesized under extreme high-pressure and high-temperature conditions such as 14-23 GPa and 2300-2500 K. In this study, we have conducted single-crystal X-ray diffraction (SC-XRD) experiments on these new phases to obtain their crystallographic and structural information.

2 Experimental Procedure

The samples of new phases have been synthesized by Zhou et al. (2018). They have called two new phases as kyanite-II (Kya-II) and kyanite-III (Kya-III). The same notation for each phase was used in this report.

Each single-crystal piece of these phase ($0.06 \text{ mm} \times 0.04 \times 0.04$ for Kya-II and $0.06 \text{ mm} \times 0.07 \times 0.02$ for Kya-III) was used for this SC-XRD experiments. This diffraction experiments were conducted with the automated X-ray diffractometer installed in the Beam Line BL-10A. The wavelength of synchrotron radiation was calibrated as $\lambda = 0.7012 \text{ \AA}$ using the unit cell volume of the standard ruby crystal (SRM1990 from National Institute of Standard and Technology). Unit cell parameters of the two phases were determined using 32- and 46- centered reflections for Kya-II and Kya-III, respectively. X-ray reflection intensity data for these phases were collected up to $2\theta_{\text{max}} = 60^\circ$ for Kya-II and 80° for Kya-III by the ω scan method (scanning time 0.5s) to determine their space group and crystal structures. Lorentz and polarization corrections were applied to all X-ray reflection data, but no corrections for crystal absorption were applied.

The structure determination of each phase was conducted. Initial structural parameters of both phases were obtained from the charge flipping method [2] with SUPERFLIP software [3]. Anisotropic displacement parameters were used for Al, Si and O atoms. Neutral atomic scattering factor of each atom specie (Al, Si and O) was taken from International Tables for Crystallography Volume C [4]. All calculations for structural refinements were performed by SHELXL97 [5] with WinGX [6].

3 Results and Discussion

The crystallographic data for these phases were obtained as follows: for Kya-II, triclinic, $a = 7.051 \text{ \AA}$, $b = 9.434 \text{ \AA}$, $c = 6.773 \text{ \AA}$, $\alpha = 96.78^\circ$, $\beta = 99.19^\circ$ and $\gamma = 108.10^\circ$; for Kya-III, monoclinic, $a = 9.294 \text{ \AA}$, $b = 4.706 \text{ \AA}$, $c = 6.626 \text{ \AA}$ and $\beta = 111.30^\circ$. The calculated densities (D_{calc}) of these phases using ideal chemical formulae were estimated as 3.877 and 3.982 ($\text{g}\cdot\text{cm}^{-3}$), respectively. Space groups of these phases were determined as $P\bar{1}$ for kyanite-II and as $C2/c$ for kyanite-III from the systematic absence rules in each X-ray reflection intensity data-set.

The structural properties of both phases are that (1) the structures are based on closed-packed oxygen arrangement, (2) there are 4- and 6- coordinated polyhedral sites for Si in the crystal structure of Kya-II, and (3) there is only 6-coordinated site for Si in the Kya-III structure.

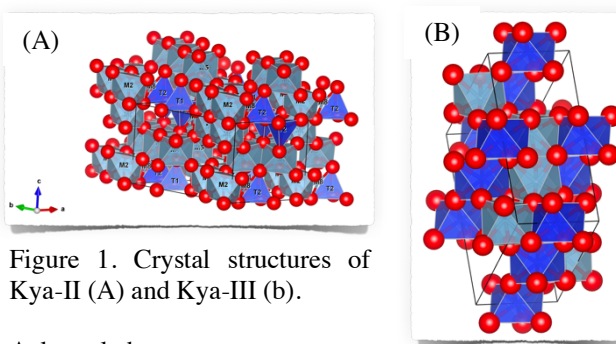


Figure 1. Crystal structures of Kya-II (A) and Kya-III (b).

Acknowledgement

The samples used for this study were given from Dr. Zhou.

References

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