Single crystal X-ray structure study of δ-phase AlOOH-FeOOH-$MgSiO_2(OH)_2$

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δ-AlOOH is an important hydrous phase for understanding the Earth’s deep water cycle, which is stable in hydrous pyrolite, hydrous basalt and hydrous sediment component of slabs subducted into the mantle transition zone and lower mantle. This phase forms a solid solution with ε-FeOOH and $MgSiO_2(OH)_2$ (Phase H). Therefore, the physical and chemical properties of δ-phase AlOOH-FeOOH-$MgSiO_2(OH)_2$ solid solution are of fundamental importance to understanding the water cycle in the deep mantle. In this study, we conducted structure analyses of δ-phase AlOOH-FeOOH-$MgSiO_2(OH)_2$ solid solution by single crystal X-ray diffraction. Single crystals of pure δ-AlOOH and δ-(Al,Fe)OOH and δ-(Al,Fe,Mg,Si)OOH with Fe, Mg and Si components up to about 10 mol% were synthesized at 21 GPa and 1480 K for 4 h using a Kawai-type multi-anvil apparatus. Single crystal structure analyses of synthetic crystals were conducted by the SHELXL-97 program. The compositions for crystal structure refinements were fixed using compositional data determined with an electron microprobe operating in wavelength-dispersive mode, in which all Fe were calculated as ferric iron. Reliability factors for each crystal were converged within 6% after the anisotropic displacement factors were refined, which indicate refined structures are reasonable. Space group of δ-AlOOH ($P2_1nm$) is not changed by substitution of Al to only Fe, whereas is changed to $Pnnm$ by addition of $MgSiO_2(OH)_2$ component. This symmetry change by $MgSiO_2(OH)_2$ components may be one of the reasons why δ-AlOOH can accommodate a large amount of $MgSiO_2(OH)_2$ component (23-44 mol%) in the deep lower mantle.

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