Determination of space group and hydrogen positions of delta-AlOOH and its relation to stishovite and brucite

Yasuhiro Kudoh[1], Takahiro Kuribayashi[2], Akio Suzuki[3], Eiji Ohtani[4], Takayuki Kamada[5]

[1] Tohoku Univ, [2] Tohoku Univ., [3] Faculty of Science, Tohoku Univ., [4] Institute of Mineralogy, Petrology, and Economic Geology, Tohoku University, [5] Geology, Tohoku Univ.

A single crystal of delta-AlOOH synthesized by Suzuki et al. (2000) at conditions of 1000 C and 21 GPa was used in this study. A set of X-ray diffraction intensities were measured with a single crystal using MoKa radiation (50 kV, 40mA). Al:Mg:Si ratio 0.84:0.07:0.09 measured by EDS with the same crystal used in the X-ray diffraction intensity measurement yielded the chemical formula (Al0.84Mg0.07Si0.09)H0.98O2. The systematic absence of reflections observed in this study indicated possible space group Pnn2 or Pnnm. The N(Z) test for a center of symmetry indicated an acentric space group. The non-centrosymmetric space group Pnn2 was therefore employed and was confirmed by the structural refinement. The agreement factors for 109 independent reflections were R=3.6% with anisotropic temperature factors. The difference Fourier synthesis was calculated and two significant Fourier peaks H1 and H2 for the possible hydrogen sites were found. The H1 site is considered to be for AlOOH and the H2 site for Mg(OH)2. The partial occupancy of Mg and Si atoms at Al site suggests the possibility of limited solid solution among delta-AlOOH, stishovite SiO2 and hypothetical rutile-structured Mg(OH)2.