Synthesis and crystal structure of a new hydrous phase delta-AlOOH

Akio Suzuki[1], Eiji Ohtani[2], Takayuki Kamada[3]

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

A new phase of AlOOH (tentatively called delta-AlOOH) was synthesized at 20.9 GPa and 1000 degree C and its crystal structure was identified by a powder X-ray diffraction method. Rietveld refinement revealed that this aluminum oxide hydroxide has a orthorhombic unit cell, a=4.7134(1)A, b=4.2241(1)A, c=2.83252(8), V=56.395 (5)A3, and Z=2 in the space group of P21nm (Rwp = 0.028, Rp = 0.021, RB = 0.074, RF = 0.046). The distribution of cations is similar to that of stishovite and CaCl2, which is the structure of the high pressure phase of stishovire. It is suggested that H is contained in SiO2 at high pressure by the substitution of Si4+ for Al3+ and H+.

A new phase of AlOOH (tentatively called delta-AlOOH) was synthesized at 20.9 GPa and 1000 degree C and its crystal structure was identified by a powder X-ray diffraction method. Rietveld refinement revealed that this aluminum oxide hydroxide has a orthorhombic unit cell, a=4.7134(1)A, b=4.2241(1)A, c=2.83252(8), V=56.395 (5)A3, and Z=2 in the space group of P21nm (Rwp = 0.028, Rp = 0.021, RB = 0.074, RF = 0.046). The distribution of cations is similar to that of stishovite and CaCl2, which is the structure of the high pressure phase of stishovire. It is suggested that H is contained in SiO2 at high pressure by the substitution of Si4+ for Al3+ and H+. A calculated density is 3.533 g/cm3 which is about 4.48 and 15.04 per cent denser than that of diaspore and boehmite, respectively. The delta-(Al0.86Mg0.07Si0.07)OOH is also stable at 20.9 GPa and 1000 degree C coexisting with majorite and phase egg, and cell parameters are a=4.710(1)A, b=4.215(1)A, c=2.839(1)A, and V=56.37(1)A3.