Structure Analysis of Hydroxyapatite by Neutron Powder Diffraction

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Hydroxyapatite (Ca10(PO4)6(OH)2) is one of the most interesting materials in current technologies due to its wide possible applications as biomaterials and electrical devices. Its physical and chemical properties relating to such uses strongly depend on the crystal structure. In particular the stability of OH ion in the structure of hydroxyapatite has been suggested to be closely related to decomposition and ionic conductivity of hydroxyapatite. The OH lattice sites have been reported to be the conduction path of hydroxyapatite and to play an important role in the proton conduction. Thus, it is important to study the position of H atoms in the hydroxyapatite. However, information of hydrogen is difficult to be detected by the powder X-ray diffraction (XRD) technique. Here, we report the structure analysis of hydroxyapatite, through a neutron powder diffraction study.

A stoichiometric hydroxyapatite sample with Ca/P=5/3 was prepared with a citric acid method. The powders were put into vanadium holder and neutron powder diffraction measurement was performed in air with a 150 detector system, HERMES, installed at the JRR-3M reactor in Japan Atomic Energy Agency, Tokai, Japan. Neutron with wavelength 1.84491 angstrom was obtained by the 331 reflection of a Ge monochromator. Diffraction data were collected in air at 298.5 K. The experimental data were analyzed by Rietveld method. A computer program RIETAN-FP was utilized for the Rietveld analysis.

Rietveld analysis of hydroxyapatite at 298.5 K was carried out assuming the P21/c space group. As shown in Fig. 1, the calculated intensities agreed well with the observed ones. The reliability factors and goodness of fit were Rwp = 5.19 %, RI = 1.16%, RF = 0.57% and S = 4.31. Lattice parameters were a = 9.4162(7) angstrom, b = 6.8789(2) angstrom, and c= 18.8685(12) angstrom. These values are consistent with the literature.

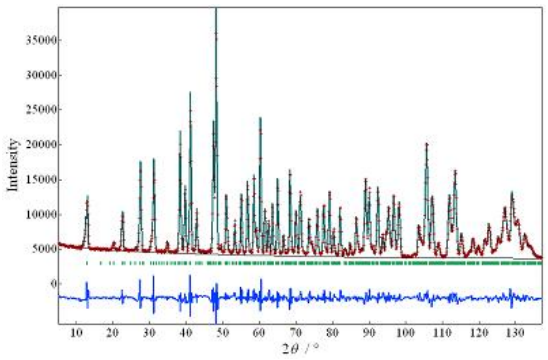

Fig. 1. Neutron powder diffraction patterns of hydroxyapatite at 298.5 K.