Crystal structure and electron density distribution of hydroxyapatite from longgu (Fossilia Ossis Mastodi) in the Kampo medicine prescription

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longgu (Fossilia Ossis Mastodi) is one of the herbal medicine, and is considered to be a fossil of a large mammal. All longgu used in Japan are imported from China. However, because it is a fossil, there is concern that natural resources will be exhausted. In this study, for the purpose of exploring alternative materials of longgu from a mineralogical point of view, we investigated the change of crystal structure accompanied by longgu in Kampo medicine prescription.
The electron density distribution of the apatite from the longgu samples were investigated by using the noisy XRD data from the laboratory instrument. For the purpose of the noise reduction for the noisy XRD data, the Savitzky-Golay filtering method (Savitzky and Golay, 1964) were applied for the XRD data. Analysis of crystal structure and electron density distribution was carried out by MEM/Rietveld method using RIETAN-FP (Izumi and Momma, 2007).
In this study, medicinal longgu of before use (rawp1), longgu was prescribed with only water (Rp1) and with other natural medicines as Kampo use (Kp1). Symbols, Rpt1and Kpt1 meen three times prescribing Rp1 and Kp1.
The XRD data were obtained by the Rigaku RAD-C Radial X-ray diffraction system. The Cu*K*a radiation with graphite monochromator was used for the measurement. The 2 theta range was from 2 degrees to 120 degrees. The measurement step was 0.02 degrees per step with the 2 seconds of fixed time. The dominant mineral phase for the longgu was identified as hydroxylapatite (HA).
The structural data and the electron density distribution data were required by investigation of the alternative materials and the evaluation of the reusability of the longgu. However, the electron density distribution by the MEM/Rietveld method in this study is considered to be insufficient accuracy for comparison with the electron density distribution by the single crystal method.
Based on the shape of the electron density distribution of PO_4 tetrahedra, it was divided into two groups <rawp1, Rpt1, Kpt1, SHA> and <Rp1, Kp1>. From this, it is considered that the structure is changed by applying Kampo medicine prescription once and that it return to the original structure when it is repeatedly prescribed. It was also confirmed that the XRD pattern of Rp1 has a different peak from that of HA.
Future tasks include increasing the accuracy of measurement of XRD patterns, identifying mineral phases with peaks different from HA of longgu's XRD pattern, and measuring and analyzing longgu of different lots.

Keywords: longgu, Kampo medicine prescription, MEM/Rietveld, hydroxyapatite

