

Structural Study on the Ferroelectric Transition in YMnO₃ by Rietveld Method

Jinyoung Kim, Nam Soo Shin* and Yang Mo Koo

Department of Materials Science and Engineering, Pohang University of Science and
Technology (POSTECH), Pohang, Korea

*Pohang Accelerator Laboratory, POSTECH, Pohang, Korea

Hexagonal YMnO₃ is one of a rare class of materials known as magnetoelectric multiferroics which are both ferroelectric and antiferromagnetic in the same phase. The origin of the ferroelectric transition at around 900K, however, has remained controversial subject of debate. To elucidate the ferroelectric distortion in this material, high resolution synchrotron x-ray powder diffraction studies have been carried out from room temperature to 1000K. Structural parameters were obtained as a function of temperature from the Rietveld refinement method. The charge density distributions of YMnO₃ in the paraelectric and ferroelectric states have been also investigated by analyzing the powder diffraction data with the maximum entropy method.