electron microscopy. Synchrotron powder diffraction data of the sample were obtained using high resolution powder diffraction beam line (8C1) at Pohang Acceleration Laboratory. In a system of (Ba1-xLax)2In2O5, two phase boundaries was existed in accordance with x, as shown in below diagram. Rietveld method was used for refining the structure parameter of the SrLaIn2O5. The cell parameters of each phase was refined as a=5.94239(2)Å, b=8.21858(3)Å, c=5.72480(2)Å for BaInO3, a=16.73045(31)Å, b=6.09718(11)Å, c=5.96295(15)Å for BaLaInO3, and a=4.15398(2)Å for (BaLa)3In2O5 respectively. The electrical conductivity of the sintered samples was measured by DC four-probe method. The relationship between the oxide-ion conductivity and crystal structure of (Ba1-xLa)xIn2O5, (0<x<1) will be discussed.

Keywords: synchrotron X-ray diffraction, Rietveld refinement, phase transitions and structure

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Synthesis and crystal structure of novel proton-conductor, RbMg(PO3)3·3(H2O)

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Proton-conductors have been devoted for applications in electrochemical devices such as fuel cells. Among these materials, proton-conductive solid acid salts, CsH2PO4 and CsHSO4, are well known as high proton conductors at medium temperature range. However, their operating temperature is narrow and the search for new proton conductors are still necessary. In the present study, a novel material with high proton conductivity was synthesized in the solid acid salt systems, and its structure was examined by X-ray and neutron diffraction measurements. New proton conductor, RbMg(PO3)3·3(H2O), was synthesized by co-precipitation method. The conductivity at intermediate temperatures was found to exceed 10−1 Scm−1. Their structures were determined by the combined neutron and x-ray Rietveld analysis from room temperature to 300℃. The PO4 tetrahedra are connected with each other by corner-sharing oxygen atoms and form the spiral-shaped chains along c-direction. Protons are found to locate at the sites around the chains, and these protons participate in the high proton conductivity. Between one-dimensional PO4 chains, these is one dimensional tunnel where water molecules situate and form a spiral chain. The deference in conduction mechanisms was observed between room temperature and high temperatures. The relationship between the structure and the proton conduction mechanism will be discussed.

Keywords: proton conductor, neutron powder diffraction, conduction mechanism

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Structural studies on lithiation process of nano-size γ-Fe2O3 using neutron scattering technique

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Iron oxides are one of the most ideal cathodes for lithium secondary batteries because of its low cost and low environmental impact, in comparison with cobalt or nickel based cathode materials. The binary iron oxide is the simplest system and was previously proposed for positive electrode materials[1]. However, an irreversible phase transformation from the corundum/spinel to the disordered rock-salt type appeared at the first lithiation process prevents reversible reactions and an application for lithium secondary batteries[1-3]. We also proposed the nano-sized crystalline γ-Fe2O3 as a lithium battery cathode materials. Lithiation mechanism of nano-size material for lithium battery electrode was studied by neutron scattering technique.