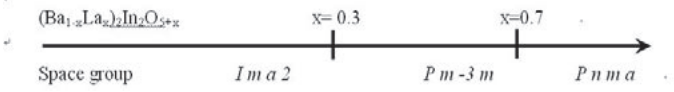
electron microscopy. Synchrotron powder diffraction data of the sample were obtained using high resolution powder diffraction beam line (8C1) at Pohang Acceleration Laboratory. In a system of $(Ba_{1-x}La_x)_2In_2O_{5+x}$, two phase boundaries was existed in accordance with x, as shown in below diagram. Rietveld method was used for refining the structure parameter of the $(Ba_{1-x}La_x)_2In_2O_{5+x}$. 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 $LaInO_3$, $a$=16.73045(31)Å, $b$= 6.09718(11)Å, $c$=5.96295(15)Å for $BaIn_2O_5$, and $a$=4.15398(2)Å for $(BaLa)In_2O_5$ 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 $(Ba_{1-x}La_x)_2In_2O_{5+x}$ (0<= x<= 1) will be discussed.




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

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### High temperature crystallographic study of perovskite-type mixed conductor, $(La_{0.5}Sr_{0.5})CoO_{3-\delta}$

Katsuhiro Nomura, Hiroyuki Kageyama
National Institute of Advanced Industrial Science and Technology (AIST), Midorigaoka 1-8-31, Ikeda, Osaka, 563-8577, Japan, E-mail：nomura-k@aist.go.jp

In this study, we aimed at elucidating the crystal structure of perovskite-type mixed conductor, $(La_{0.5}Sr_{0.5})CoO_{3-\delta}$ (LSC) at high temperatures under controlled oxygen partial pressures, $P(O_2)$. The LSC sample was synthesized by a coprecipitation method. High temperature X-ray diffraction (HT-XRD) measurements were carried out under the following experimental conditions: Cu-K$\alpha$ radiation, a parallel-beam optics, 298 $\leq T \leq$ 1173K, $2\times10^{-3} \leq P(O_2) \leq$ 0.21 atm). The XRD data were refined by the Rietveld method using the computer program RIETAN-2000. The XRD patterns could be indexed as a trigonal perovskite unit cell ($R$-3$c$) from 298 to 373K under $P(O_2)$ = 0.21atm, and as a cubic one ($Pm$-3$m$) from 473 to 1173K under $P(O_2)$ range from $2\times10^{-3}$ to 0.21atm. Electron density distribution analysis of the XRD data of LSC was carried out by a combination of Rietveld analysis, the maximum-entropy method (MEM), and MEM-based pattern fitting (MPF) using the computer program PRIMA. Electronic states and local structures of metal ions in LSC were analyzed by X-ray absorption fine structure (XAFS). The La K- and Sr K-XAFS of the LSC were measured at 295K-in air, 996K-in air, 1vol%$O_2$-$N_2$, and $N_2$ using the beam line BL01B1 of SPring-8. The Co K-XAFS of the LSC was measured at 295K-in air, 923K-in air, 1vol%$O_2$-$N_2$, and $N_2$ using laboratory equipment EXAC-820 (Technos Co., Ltd.). The peak intensity at around 16.11keV of the Sr K-edge decreased with increasing temperature and decreasing $P(O_2)$, suggesting that Sr-O interactions (i.e. chemical bonds) decreases under these conditions. While the Co K-edge shifted to lower energy with increasing temperature and decreasing $P(O_2)$, suggesting that Co-O interactions (i.e. chemical bonds) decreases under these conditions.

Keywords: perovskite oxides, high-temperature diffractometry, XAFS

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### Synthesis and crystal structure of novel proton-conductor, $RbMg(PO_3)_3\cdot3(H_2O)$

Masao Yonemura[1], Hikaru Koga[2], Cedric Pitteloud[2], Hiromasa Iyama[2], Yasuaki Matsuda[2], Daisuke Mori[2], Miki Nagao[2], Atsuo Yamada[2], Ryoji Kanno[2]
[1]Ibaraki University, 4-12-1 Nakanarusawa, Hitachi, Ibaraki, 316-8511, Japan, [2]Tokyo Institute of Technology, 4259 Nagatsuta, Midori, Yokohama, Kanagawa, 226-8502 Japan, E-mail：yonemura@mx.ibaraki.ac.jp

Proton-conductors have been devoted for applications in electrochemical devices such as fuel cells. Among these materials, proton-conductive solid acid salts, $CsH_2PO_4$ and $CsHSO_4$, 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, $RbMg(PO_3)_3\cdot3(H_2O)$, was synthesized by co-precipitation method. The conductivity at intermediate temperatures was found to exceed $10^{-3}$ $Scm^{-1}$. Their structures were determined by the combined neutron and x-ray Rietveld analysis from room temperature to 300°C. The $PO_4$ 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 $PO_4$ 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 $\gamma$-$Fe_2O_3$ using neutron scattering technique

Miki Nagao[1], Sho Kanzaki[1], Joe Fleramosca[3], Ryoji Kiyanagi[3], Keiji Itoh[4], Masao Yonemura[2], Atsuo Yamada[1], Ryoji Kanno[1]
[1]Tokyo Institute of Technology, Interdisciplinary Graduate School of Science and Engineering, 4259-G1-01 Nagatsuta-cho, Midori-ku, Yokohama, kanagawa, 226-8502, Japan, [2]Ibaraki University, 4-12-1 Nakanarusawa, Hitachi, Ibaraki, 316-8511, Japan, [3]Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439, United States of America, [4]Kyoto University, Kumatori-cho, Sennan-gun, Osaka 590-0494, Japan, E-mail：nagao@echem.titech.ac.jp

Iron oxides are one of the most ideal cathodes for lithium secondly 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 $\gamma$-$Fe_2O_3$ as a lithium battery cathode materials. Lithiation mechanism of nano-size material for lithium battery electrode was studied by neutron scattering technique.