Poster Presentation

MS79.P05

In situ synchrotron powder diffraction for an ionic conductor transition

H. Kasai[1,2], K. Kato[1,2], A. Hori[1], M. Takata[1], S. Kitagawa[1,3], H. Tanaka[4], H. Arikawa[2,5], T. Takeguchi[2,5], M. Sadakiyo[2,6], M. Yamauchi[2,6]
[1]RIKEN SPring-8 Center, Hyogo, Japan, [2]JST, CREST, Saitama, Japan, [3]Kyoto University, Kyoto, Japan, [4]Shimane University, Matsue, Japan, [5]Iwate Univniversity, Morioka, Japan, [6]Kyushu University, Fukuoka, Japan

In situ synchrotron X-ray powder diffraction can be one of the most powerful probes to investigate the structure evolution by a chemical reaction thanks to simultaneity of data collection. It is not, however, with ease to produce a homogeneous chemical reaction in the limited spaces, which is essential to see an atomic-scale structure evolution. We have developed an in situ capillary cell for both high-temperature H_2 reduction and precise humidity control at the SPring-8 BL44B2. We successfully applied this in situ system to an electronic conductor $LaSr_3Fe_3O_{10}$, which is transformed into an ionic conductor by the two-step chemical treatments [1]. $LaSr_3Fe_3O_{10}$ has a triple-layer structure with a FeO_6 octahedral unit. One triple layer is bonded with another layer through van der Waals interaction. Structure refinements with in situ synchrotron powder diffraction data revealed that the H_2 reduction at 613 K produced in-plane oxygen vacancies, which resulted in suppression of the interlayer interaction. We found from charge density studies and Raman spectroscopy measurements that the following humidification intercalated H_2O and OH^- into the interlayer and intralayer, respectively. That means that H_2O plays a role for suppression of three-dimensional electronic conductivity, stabilizing the intercalation structure. On the other hand, the OH^- ions behave as carriers for ionic conductivity, maintaining the charge neutrality in the intralayer. Finally we determined the composition of the ionic conductor to be $LaSr_3Fe_3O_{8.0}(OH)_{12}\bullet 2H_2O$, which indicates a transformation of $LaSr_3Fe_3O_{10}$ into an OH^- ionic conductor. In the presentation, I will discuss the OH^- ionic conduction channel based on electrostatic potentials obtained from charge densities.

[1] *T. Takeguchi et al., J. Am. Chem. Soc. 2013, 135, 11125-11130.*

Keywords: In situ synchrotron X-ray powder diffraction, Layered oxide, Ionic conductor