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Masatomo Yashima

Tokyo Institute of Technology, Japan

Visualization of the ion-diffusion path and chemical bonding in inorganic materials

Ion diffusion and chemical bonding in solid materials are important in various research fields of chemistry, physics and pharmacy. Our group has developed new high-temperature neutron and high-resolution synchrotron X-ray diffraction techniques to study the precise crystal structures, nuclear and electron densities in inorganic materials from room temperature to 1900 K. Bond valence method is useful to examine the crystal structure and ion diffusion paths. These techniques enabled precise structure analysis leading to the ion-diffusion path, chemical bonding and structural disorder in ionic conductors. In the present keynote speech, we present the diffusion path and/or chemical bonding of mobile ions in Bi_2O_3, $Bi_{1.4}Yb_{0.6}O_3$, $(La_{0.8}Sr_{0.2})$, $(Ga_{0.8}Mg_{0.15}Co_{0.05})O_{3-\delta}$, CeO_2, $Ce_{0.93}Y_{0.07}O_{1.96}$, $PrBaCo_2O_{5+\delta}$, $(Pr_{0.9}La_{0.1})_2(Ni_{0.74}Cu_{0.21}Ga_{0.05})O_{4+\delta}$, $Pr_2(Ni_{0.75}Cu_{0.25})_{0.95}Ga_{0.05})$-$O_{4+\delta}$, and biomaterial hydroxyapatite at high temperatures. We synthesized and discovered novel materials $BaNdInO_4$ and $SrYbInO_4$ and their crystal structures were determined by synchrotron X-ray and neutron powder diffraction and *ab initio* electronic calculations. As these materials exhibit oxide-ion conduction, we have discovered new structure families of oxide-ion conductors $BaNdInO_4$ and $SrYbInO_4$. The bond valence sum (BVS) map of $BaNdInO_4$ and bond valence-based energy landscape of $SrYbInO_4$ at 1000°C strongly suggested two-dimensional and one-dimensional oxide-ion diffusion, respectively. Sr and Ba substitutions at the Nd site improve the oxide-ion conductivity of $BaNdInO_4$. Careful structure analyses using both the single-crystal X-ray diffraction and time-of-flight neutron powder diffraction data of $Ba_{1.1}Nd_{0.9}InO_{3.95}$ enabled to determine the position of excess Ba cation and occupancy factor of O anion. The present findings might open a new window in chemistry, physics and pharmacy.

Biography

Masatomo Yashima obtained his PhD in Materials Science and Engineering from Tokyo Institute of Technology, Japan in 1991. He has been a Full Professor at the institute from April 2011 to present. He was also a Research Associate and an Associate Professor at the same institute. He has published over 500 papers, including over 212 original research papers (cited over 10297 times (Google Scholar, Feb. 28, 2018). He has received over 28 awards including CSJ Award for Creative Work (2018), Award of the Ceramic Society of Japan (2009), the Award of the Crystallographic Society of Japan (2008).

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yashima@cms.titech.ac.jp

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