Department of Quantum Materials
Max Planck Institute for Solid State Research

The Sir Martin Wood Prize Lecture

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Creation of hydride super-ionic conductors

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Biography

2006 B.Eng. Department of Chemistry and Chemical Engineering, Kanazawa University

2008 M.Eng. Department of Electronic Chemistry, Tokyo Institute of Technology

2010 Ph.D. Department of Electronic Chemistry, Tokyo Institute of Technology

2010 Postdoctoral Fellow, Department of Electronic Chemistry, Tokyo Institute of Technology

2011 Assistant Professor, Department of Material and Life Chemistry, Kanagawa University

2012 JST-PRESTO Researcher

2013 Research Associate Professor, Institute for Molecular Science, National Institutes of Natural Sciences

2018 Associate Professor, Institute for Molecular Science, National Institutes of Natural Sciences

2018 Associate Professor, The Graduate University for Advanced Studies

2022 Chief Scientist, Solid State Chemistry Laboratory, Cluster for Pioneering Research, RIKEN

2022 Professor, Institute for Molecular Science, National Institutes of Natural Sciences

SIR MARTIN WOOD PRIZE LECTURE

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MPI for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart (Germany)

Hydrogen can become a positively charged proton (H^+) to a negatively charged hydride ion (H^-) through the exchange of electrons in the 1s orbital. The charge flexibility allows hydrogen to exist in a wide variety of materials while changing its charge and size; however, H^- is usually stable only when it forms hydrides with alkali metals and alkaline earth metals with low electronegativity. In fact, the diffusion of hydrogen in solids in fuel cells, hydrogen sensors, and hydrogen storage alloys, which are fundamental techniques for hydrogen energy utilization, has mostly been related to the diffusion of H^+ or atomic hydrogen (H^0), and H^- has not been recognized as a movable ion for a long time. In the 2000s, it was found that significant concentrations of H^- could be introduced into oxides, and mixed-anion compounds, in which H^- could be relatively stable began to be developed. The main aim was to explore new physical properties and catalytic functions by utilizing the electron-donating properties of H^-. On the other hand, we considered H^- to be a promising charge carrier for electrochemical devices including batteries, fuel cells, and electrolysis cells because hydride ions have not only properties suitable for fast ionic conduction, such as monovalent, moderate ionic radius, and high polarizability, but also a strong reducing ability (–2.25 V vs. SHE). To create electrochemical devices with a new operation principle based on the above-mentioned features of H^-, we have been developing H^- conductors, which had been practically unexplored.

By adding alkali metals and alkaline earth metals with low electronegativity, which can stabilize the H^- charge state, to the constituent elements, we created a series of oxyhydride system, $(La_{2-x-y}Sr_{x+y})\ LiH_{1-x+y}O_{3-y}$,that shows pure H^- conductivity without any contribution from electron conduction (transporter number $t_H = 1$). As a result of expanding the material system of H^- conductors based on this achievement, we achieved the creation of $Ba_{1.75}LiH_{2.7}O_{0.9}$ (BLHO), exhibiting high H^- conductivity above 10^{-2} S·cm^{-1} through phase transition. BLHO is 20% deficient in H^- within the H^- diffusion layer, and at room temperature, this defect orders to form a superlattice. With increasing temperature, the long-range ordering of the H^- defects disappeared, which triggered a nearly temperature-independent high conductivity above 10^{-2} S·cm^{-1}. This conduction behaviour is unique to super-ionic conductors in which mobile ions are in collective motion, showing that BLHO is a H^- superionic conductor. Furthermore, we recently demonstrated that elemental substitution into BLHO effectively lowers the phase transition temperature and improves conductivity in the low-temperature region. There remains room for further performance improvements, such as optimization of the substituted species and their concentrations and multi-element substitution; thus, stabilization of the highly conductive phase of BLHO would be a principal guideline for developing hydride ion conductors.

Dr. Kobayashi was awarded the Sir Martin Wood Prize at the Millennium Science Forum which took place in November 2023. The Millennium Science Forum was established in 1998 to promote scientific exchange between Britain and Japan and recognize the work of outstanding young Japanese researchers. The prize is named after Sir Martin Wood, founder of Oxford Instruments.