Development of Hydride Ion Conductors

Genki Kobayashi : Institute for Molecular Science, Ryoji Kanno : Tokyo Institute for Technology

Hydrogen transport in solids is key for determining the performance of electrochemical devices such as fuel cells and batteries. Indeed, active studies on proton (H^+) conduction in oxides and other systems have been carried out to date. In contrast, hydrogen can also accept one electron to form hydride (H^-). The conduction of hydride ions is attractive because these have an ionic radius appropriate for fast ionic conduction and also show strong reducing properties with a standard redox potential of H^-/H_2 (–2.3 V), which is close to that of Mg/Mg^{2+} (–2.4 V). Hydride ion conductors may therefore be applied in energy storage/conversion devices with high energy densities. However, pure H^- conduction has been verified only for a few hydrides of alkaline earth metals such as BaH_2 [1]. Unfortunately, utilization of the hydrides is difficult because of their structural inflexibility, which makes control of the lattice structure to create smooth transport pathways and control of the conducting hydride ion content difficult. We have considered oxyhydrides, where hydride ions and oxide ions share the anion sublattices, as candidate hydride conductors equipped with flexible anion sublattices.

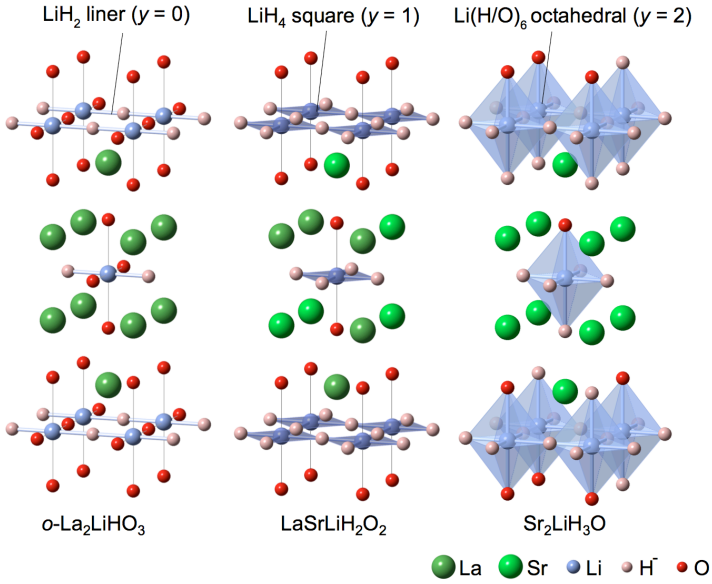

Fig. 1. Crystal structure of $La_{2-x-y}Sr_{x+y}LiH_{1-x+y}O_{3-y}$ (x = 0, y = 0, 1, 2)

Recently, we developed a series of K_2NiF_4-type oxyhydrides, $La_{2-x-y}Sr_{x+y}LiH_{1-x+y}O_{3-y}$, which are equipped with anion sub-lattices that exhibit flexibility in the storage of H^-, O^{2-}, and vacancies (Fig. 1) [2,3]. The oxyhydride system exhibited a pure H^- conductivity of 10^{-4} S cm^{-1} at 300 °C. Furthermore, the all-solid-state $Ti/La_{2-x-y}Sr_{x+y}LiH_{1-x+y}O_{3-y}/TiH_2$ cell exhibited a redox reaction with hydrogen storage/desorption on the electrodes. The present success in the construction of this all-solid-state electrochemical cell exhibiting H^- diffusion confirms not only the capability of the oxyhydride system to act as a solid hydride electrolyte, but also the possibility of developing electrochemical solid devices based on H^- conduction for the first time.

Bibliography

[1] M. C. Verbraeken, J. T. S. Irvine *et al.*, *Nat. Mater.,* **14**, 95-100 (2015).

[2] G. Kobayashi, M. Yonemura, I. Tanaka, R. Kanno *et al.*, *Science*, **351**, 1314 (2016).

[3] A. Watanabe, G. Kobayashi *et al.*, *Electrochemistry*, **85(2)**, 88-92 (2017).