New materials with high oxygen-ion conductivity opening sustainable future

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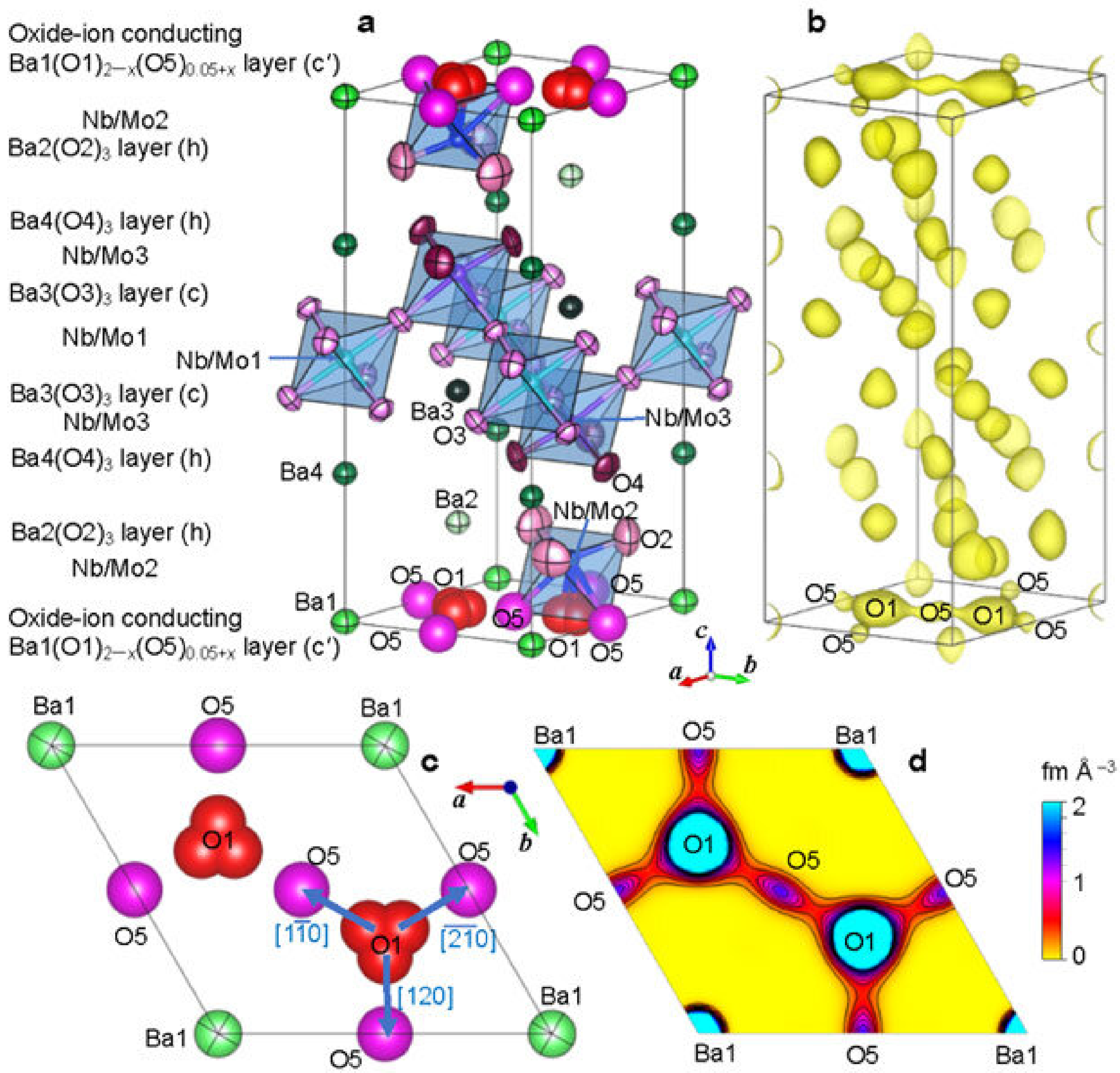


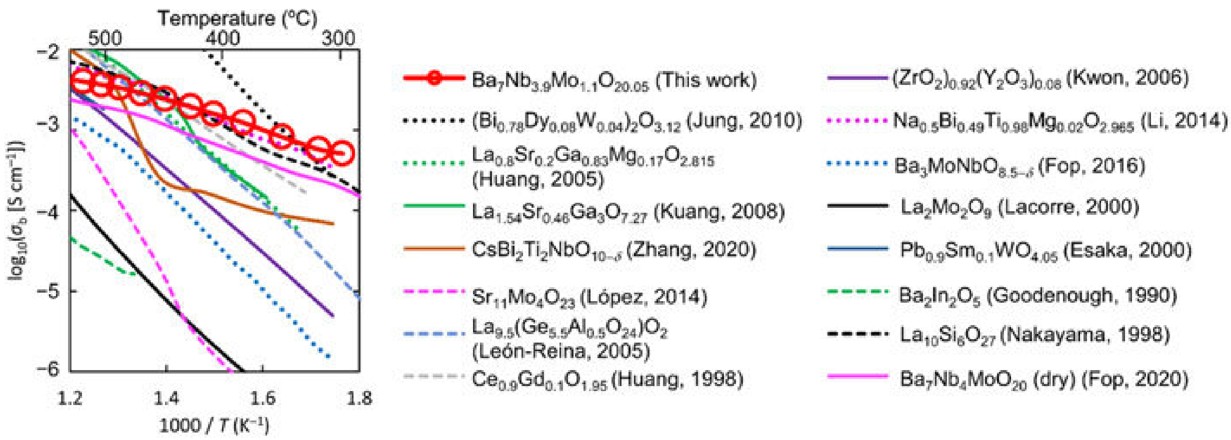
Experimental evidence of the interstitial oxygen O5 and the O1−O5 oxide-ion interstitialcy diffusion of Ba7Nb3.9Mo1.1O20.05 at a high temperature of 800 oC. Credit: Tokyo Institute of Technology

Scientists at Tokyo Institute of Technology (Tokyo Tech), Imperial and High Energy Accelerator Research Organization (KEK) Institute of Materials Structure Science, discover new $Ba_7Nb_4MoO_{20}$-based materials with high oxygen-ion (oxide-ion O^{2-}) conductivities—"the hexagonal perovskite-related oxides"—and shed light on the underlying mechanisms responsible for their conductivity. Their findings lead the way to uncovering other similar materials, furthering research on developing low-cost and scalable renewable energy technologies.

Over the past few years, fuel cells have become a focal point of research in eco-friendly technology because of their superior abilities to store and produce renewable energy and clean fuel. A typical type of fuel cell gaining ground is the oxide-ion-conducting fuel cell, which is primarily made of materials through which oxide ions (oxygen ions: O^{2-}), can easily move. New materials with higher conductivity at low and intermediate temperatures, provide a number of advantages over commonly used fuel cells based on yttria-stabilized zirconia (YSZ) electrolytes, such as higher power generation efficiency, longer lifetimes, and lower costs.

However, only a limited number of such materials are known and their application to developing fuel cells has largely remained at the laboratory scale. To truly achieve a sustainable energy economy, new oxide-ion conductors with high conductivity need to be discovered that can allow low-cost and efficient scaling up of these technologies.

Scientists from Tokyo Tech, Imperial and KEK set out to address this need, and in a recent study, identified a new oxide-ion-conducting material that may be a representative of an entire family of oxide-ion conductors.



Comparison of bulk conductivities σb of Ba7Nb3.9Mo1.1O20.05 and other oxide-ion conductors. Credit: Tokyo Institute of Technology

The material in question has the chemical formula $Ba_7Nb_{3.9}Mo_{1.1}O_{20.05}$ and is classified as a "hexagonal perovskite-related oxide." Prof Masatomo Yashima, who led the study, explains: "$Ba_7Nb_{3.9}Mo_{1.1}O_{20.05}$ shows a wide stability range and predominantly oxide-ion conduction in the oxygen partial pressure range from $2x10^{-26}$ to 1 atm. Surprisingly, bulk conductivity of $Ba_7Nb_{3.9}Mo_{1.1}O_{20.05}$, 5.8×10^{-4} S/cm, is remarkably high at 310 °C, and higher than bismuth oxide- and zirconia-based materials. Prof Stephen Skinner comments that the fast oxide ion transport was unambiguously confirmed using the ^{18}O tracer diffusion technique at Imperial.

Prof Yashima and his team note that the crystal structure of $Ba_7Nb_{3.9}Mo_{1.1}O_{20.05}$ contains oxygen-deficient layers, and that its high oxide-ion conductivity is attributable to the oxide-ion migration on the c' layers. In fact, they succeed in experimental visualization of O1-O_5 oxide-ion diffusion pathways by the neutron-diffraction measurements at a high temperature 800 oC with SuperHRPD diffractometer of Prof Takashi Kamiyama's group at KEK/J-PARC. Prof Yashima says that the oxide ions migrate via interstitialcy diffusion mechanism through interstitial octahedral O5 and lattice tetrahedral O1 oxygen sites and that the (tetrahedral)-(octahedral) diffusion pathways on the c' layer in $Ba_7Nb_{3.9}Mo_{1.1}O_{20.05}$ is the same as those in another hexagonal perovskite-related oxide $Ba_3MoNbO_{8.5-\delta}$. Therefore, Prof Yashima and his team claim that "The common feature of the diffusion mechanism would be a guide for design of oxide-ion conductors with the hexagonal perovskite related structures and that the present finding of high oxide-ion conductivities in rare-earth-free $Ba_7Nb_{3.9}Mo_{1.1}O_{20.05}$suggests the ability of various hexagonal perovskite related oxides as superior oxide-ion conductors."

More information: Masatomo Yashima et al. High oxide-ion conductivity through the interstitial oxygen site in Ba7Nb4MoO20-based hexagonal perovskite related oxides, *Nature Communications* (2021). DOI: 10.1038/s41467-020-20859-w

Provided by Tokyo Institute of Technology