Researchers probe invisible vacancies in fuel cell materials

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(Phys.org) -- Knowing the position of missing oxygen atoms could be the key to cheaper solid oxide fuel cells with longer lifetimes. New microscopy research from the Department of Energy's Oak Ridge National Laboratory is enabling scientists to map these vacancies at an atomic scale.

Although fuel cells hold promise as an efficient energy conversion technology, they have yet to reach mainstream markets because of their high price tag and limited lifespans. Overcoming these barriers requires a fundamental understanding of fuel cells, which produce electricity through a chemical reaction between oxygen and a fuel. As conducting oxygen ions move through the fuel cell, they travel through vacancies where oxygen atoms used to be. The distribution, arrangement and geometry of such oxygen vacancies in fuel cell materials are thought to affect the efficiency of the overall device.

"A big part of making a better fuel cell is to understand what the oxygen vacancies do inside the material: how fast they move, how they order, how they interact with interfaces and defects," said ORNL's Albina Borisevich. "The question is how to study them. It's one thing to see an atom of one type on the background of atoms of a different type. But in this case, you want to see if there are a few atoms missing. Seeing a void is much more difficult."

In research published in Nature Materials, ORNL scientists used scanning transmission electron microscopy to determine the distribution of oxygen vacancies in a fuel cell cathode material below the level of a single unit cell. The team verified its findings with theoretical calculations and neutron experiments at the lab's Spallation Neutron Source.

"Even though the vacancy doesn't generate any signal in the electron micrograph, it's still a big disturbance in the structure," Borisevich said. "You can see that the lattice expands where vacancies are present. So we tracked the lattice expansion around vacancies and compared it with theoretical models, and we were able to develop a calibration for this type of material."

By providing a means to study vacancies at an atomic scale, the ORNL technique will help inform the development of improved fuel cell technologies in a systematic and deliberate fashion, in contrast to trial and error approaches.

Beyond its relevance to applications in fuel cells and information storage and logic devices, ORNL coauthor Sergei Kalinin explains that the team's research is also building a bridge between two scientific communities that traditionally have had little in common.

"From my perspective, it is physics marrying electrochemistry," Kalinin said. "The idea is that vacancies are important for energy, and vacancies are important for physics. The materials that physicists like to study are exactly the same as the materials used for fuel cells, and unless we understand how vacancies behave at interfaces, ferroic domain walls, and in thin films, we will not be able to fully appreciate the physics of these systems."

The team's research is also reinforced by a parallel study published in Physical Review Letters, with Borisevich and Kalinin as coauthors, that explains how to obtain parameters that describe vacancy-ordered systems from electron microscopy data.

Provided by Oak Ridge National Laboratory