

Unlocking the Secrets of Titanium, a 'Key' that Assists Hydrogen Storage

July 24 2004

New research may lead to better catalysts for hydrogen fuel cells

Scientists at the U.S. Department of Energy's Brookhaven National Laboratory and the New Jersey Institute of Technology have taken steps toward understanding how a titanium compound reacts with a hydrogenstorage material to catalyze the release and re-absorption of hydrogen. Their results, appearing in the July 19, 2004, issue of Applied Physics Letters, may help scientists learn how similar catalysts work, improve their performance, and possibly develop more efficient storage materials for hydrogen fuel cells.

In the late 1990s, scientists discovered that adding, or "doping," a small amount of titanium to sodium aluminum hydride, a hydrogen storage compound (also known as sodium alanate), allows it to reversibly release and re-absorb hydrogen. In a sense, the titanium acts like a molecular "key," a crucial component that facilitates hydrogen absorption and allows the reaction to proceed more rapidly. Until now, however, the nature of that reaction was not well understood.

"We found that the titanium resides on the surface of sodium alanate as a titanium aluminum compound called titanium aluminide, rather than entering the bulk material and replacing other atoms or occupying empty spots within the lattice," said the study's lead author, Brookhaven physicist Jason Graetz.

To make their finding, Graetz and his collaborators first prepared two



titanium-doped samples by mechanically mixing titanium chloride and sodium alanate using a planetary mill, a device that grinds substances together using marble-sized metal spheres. They then prepared two additional samples from each doped sample (for a total of six): a dehydrided sample (containing no absorbed hydrogen) and a hydrided sample. By working with both types, the researchers were able to study the titanium's properties before and after hydrogen absorption. This gave them one more way to determine the titanium's role in the reaction.

The group probed the samples with high-energy <u>x-rays</u> at the National Synchrotron Light Source at Brookhaven, a facility that produces intense beams of x-ray, ultraviolet, and infrared light for research. Because every compound and element on Earth absorbs x-rays differently, having a unique "signature," the researchers were able to compare the six sample signatures to those of different titanium compounds and pure titanium. From this, they determined that the titanium chloride reacted with sodium alanate to form titanium aluminide.

"Our finding is the first step toward an even more interesting discovery: determining exactly how titanium aluminide helps the hydride release and re-absorb hydrogen," Graetz said. "Understanding that mechanism may help us identify better catalysts for the sodium alanate system and help us find dopants for new compounds that are currently impractical energy-storage materials, due to the high temperatures and pressures required for the release and re-absorption of hydrogen."

Sodium alanate is one of several metal-based hydrogen storage materials, called metal hydrides, being investigated for use in hydrogen fuel cells. A fuel cell works like a battery: Hydrogen atoms enter the negative terminal and split into their constituent particles, protons and electrons. The protons pass through the cell to the positive terminal, while the electrons leave the cell as a stream of electric current that can power a car or appliance, for example. The electrons then re-enter the cell at the



positive terminal and reunite with the protons and oxygen to form water molecules.

The known hydrides are impractical for fuel cells, which require lightweight materials with high storage capacities, because they are quite heavy and have relatively low storage capacities (less than five percent hydrogen by weight). However, they have more potential than compressed hydrogen gas or liquid hydrogen, which pose explosion and freezing risks. These forms of hydrogen must be stored in tanks under very high pressure or at temperatures cold enough to liquefy the oxygen in air.

This research was funded by Brookhaven's Laboratory Directed Research and Development (LDRD) Program and the National Science Foundation.

Source: Brookhaven National Laboratory

Citation: Unlocking the Secrets of Titanium, a 'Key' that Assists Hydrogen Storage (2004, July 24) retrieved 28 April 2024 from <u>https://phys.org/news/2004-07-secrets-titanium-key-hydrogen-storage.html</u>

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