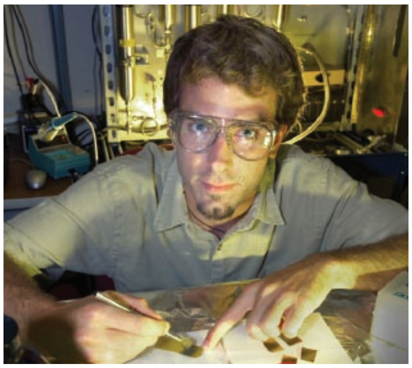
Unlocking the Secrets of Titanium, a “Key” that Assists Hydrogen Storage

New research may lead to better catalysts for hydrogen fuel cells

Scientists at Brookhaven National Laboratory and the New Jersey Institute of Technology have taken steps toward understanding how a titanium compound reacts with a hydrogen-storage 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.



Jason Graetz

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” that facilitates hydrogen absorption and allows the reaction to proceed more rapidly. Until now, however, the nature of that reaction was not well understood.

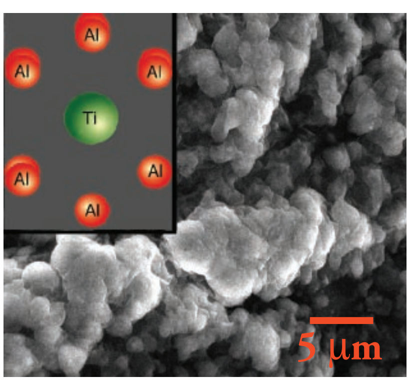
“We found that the titanium resides on the surface of sodium alanate as a titanium aluminum compound called titanium aluminide, rather than entering the bulk material and replacing other atoms or occupying empty spots within the lattice,” said the study’s lead author, Brookhaven physicist Jason Graetz.

Graetz and his collaborators first prepared two titanium-doped samples by 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 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 x-rays at the National Synchrotron Light Source (NSLS) beamline X19A. Because every substance 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 to release and re-absorb 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. The electrons then re-enter the cell at the positive terminal and reunite with the protons and oxygen to form water molecules.



Scanning electron microscope image of Ti-doped sodium aluminum hydride.

The known hydrides are impractical for fuel cells 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.

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—Laura Mgrdichian