Shaking up the Hydrogen Fuel Race

BY KERRY GIBSON

THE CONCEPT SEEMS SIMPLE. YOU PUT TWO compounds into a steel container, add some stainless steel ball bearings, tighten down the lid, then shake the heck out of it. When you open the container, the two compounds have undergone a transformation, creating new compounds that normally require the use of a solvent.

Ames Laboratory scientist Vitalij Pecharsky has been studying "mechanochemistry" for more than a decade to unlock the secret of how ball-milling is able to facilitate important solid state reactions at room temperature without the use of solvents.

"Because of the process – stainless steel balls smashing together inside a sealed stainless steel container – you can't probe the materials while you process them," Pecharsky says. "The best you can do is take samples periodically and hope to develop a map for what's taking place."

While solvent-free mechanochemical processing could revolutionize industries across the spectrum, Pecharsky and his Ames Lab colleagues have focused most of their attention on aluminum trihydride (AlH_3, also known as alane) because of its potential as a hydrogen fuel source. Alane shows promise because it can safely store and distribute large amounts of hydrogen confined in a solid material and it releases its hydrogen at a relatively low temperature so it doesn't require much input energy. It can also be used as a solid propellant, such as rocket fuel, with both the hydrogen and aluminum consumed as fuel.

As a fuel, hydrogen has about three times more energy than gasoline by weight. However, for a car to carry an equivalent amount of hydrogen fuel as a typical tank of gasoline, it would have to be stored at extremely high pressure or liquified at -253 degrees Celsius, neither of which is economically or commercially feasible. Storing hydrogen as a solid material offers the auto industry a more practical alternative.

To produce AlH_3, Shalabh Gupta and Ihor Hlova – members of the team – place an alkali metal hydride, such as lithium hydride, sodium hydride or potassium hydride in a ball mill with an aluminum halogenide, such as aluminum chloride, aluminum bromide or aluminum iodide.

"If you start with lithium hydride (LiH) and aluminum chloride ($AlCl_3$) and mill them together, you wind up with LiCl and AlH_3," Pecharsky says. "You don't lose anything and it doesn't require a solvent. We can get the same results using sodium hydride, which is much more readily available. So it can be relatively inexpensive to produce; you don't have waste other than LiCl or NaCl (common kitchen salt) or used solvent to dispose of."

Importantly, it doesn't require a lot of energy to break AlH_3 into its individual components. According to Pecharsky, it degrades into aluminum and hydrogen at about 100 degrees C – the boiling point of water.

"The Department of Energy has set targets for hydrogen production systems at six percent by weight by the year 2015," he says. "Our technique is capable of producing a total hydrogen capacity of 10 percent so we're optimistic about its potential."

Besides Pecharsky's group's experimental work, other Ames Lab scientists are involved in the project. Characterization by solid-state NMR (nuclear magnetic resonance) expert Marek Pruski and his group members – Takeshi Kobayashi and Jennifer Goldston, and microscopist Scott Chumbley and his student Tim Prost are helping to unlock what is taking place inside the ball mill. And theorist Duane Johnson and members of his team – LinLin Wang and Nikolai Zarkevich – are working to understanding the how. The work is being funded by DOE's Office of Basic Energy Sciences.

One Scientist, Several Hats

"My basic training, going all the way back to the 70s was in chemistry," says Pecharsky, who received his B.S. and M.S. degrees in chemistry and his Ph.D in inorganic chemistry all from L'viv State University in L'viv, Ukraine. "But later on, I switched to materials science and then physics, so I don't really know who or what I am anymore."

He came to Ames Laboratory and Iowa State University in 1993 as a visiting scientist, working with Karl Gschneidner Jr. on magnetic refrigeration and stayed on full time in 1995. His involvement in the hydrogen research came about as a result of scientific curiosity.

"How did I get involved in this? That's probably the million dollar question," Pecharsky chuckles. "There are two things that we look at; one is the science and the second is potential practical application – do we have a useful product at the end."

"The science here is very interesting because there's little you can do to characterize the materials during the process," he adds. "You monitor them at various points and then try do deduce what's taking place. But it's that difficulty that makes it interesting. Advanced characterization and strong theoretical support help a lot."

"Together with my former colleague – Dr. Viktor Balema, who is now with Sigma Aldrich – we initiated an exploratory effort related to mechanochemistry of complex hydrides more than 15 years ago," says Pecharsky. "And today we have a useful process that leads to alane, as described in our recent provisional patent application filed with the U.S. Patent and Trademark Office."

Shalabh Gupta holds a ball mill canister where the solvent-free reaction takes place. The sealed canister presents challenges to understanding just how the reaction is carried out.