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Regional University Alliance

NEWS

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Liberating Hydrogen: Creating the Fuel of the Future with Metallic Membranes

As our energy requirements grow, hydrogen—the lightest and most common element on earth—has become an attractive alternative fuel source. It is used to power fuel cells in a process that generates electricity from oxygen and hydrogen, producing environmentally-friendly water vapor in the process. Hydrogen gas (H_2) is also useful in chemical industries, the food industry, and fossil-fuel processing.

Although abundant, finding hydrogen in its pure elemental form is rare. Instead, we produce it by separating it from hydrogen-containing gas mixtures created during catalytic and chemical manufacturing processes. Syngas, the end-product of coal gasification, is one of those mixtures. Syngas contains methane, carbon monoxide, carbon dioxide (CO_2), and other components that often include hydrogen sulfide, arsenic, and selenium. While hydrogen-separating membranes are commercially available, historically they haven't been able to hold up to corrosion caused by the contaminants, so separation options have not been cost-effective for syngas.

Researchers with the National Energy Technology Laboratory Regional University Alliance's (NETL-RUA) Hydrogen and Clean Fuels Project hope to solve that problem by focusing on creating unique palladium (Pd)-alloy membranes that selectively separate hydrogen from syngas and resist corrosion. "For a membrane to be successful, it has to first dissociate H_2 into hydrogen atoms," explains **Dirk Link**, technical coordinator for the NETL-RUA Fuels team. Palladium is a catalyst, driving H_2 molecule dissociation into pure hydrogen atoms that are capable of diffusing through the membrane. Those atoms recombine into H_2 gas after passing through the membrane. But as Link noted, "if the surface of the membrane corrodes, catalytic dissociation stops, and you're sunk." That corrosion also has a detrimental effect on diffusion of the hydrogen atoms.

>> *See* **METALLIC MEMBRANES**, *Page 2*

What's in This Issue

NETL-RUA Research Project Seeks to Protect Alloys in Harsh Environments . . . . . p. 2

No Structure Too Big, No Device Too Small: SBEUC Helps NETL-RUA Researchers Run Simulations at Various Scales . . . . . p. 3

Under Pressure: ORISE Postdoctoral Researcher Works with NETL Scientists to Develop Membrane System for Carbon Dioxide Separations. . . . . p. 4

Researchers Poised to Patent Advanced Gas Sensor. . . . . p. 4

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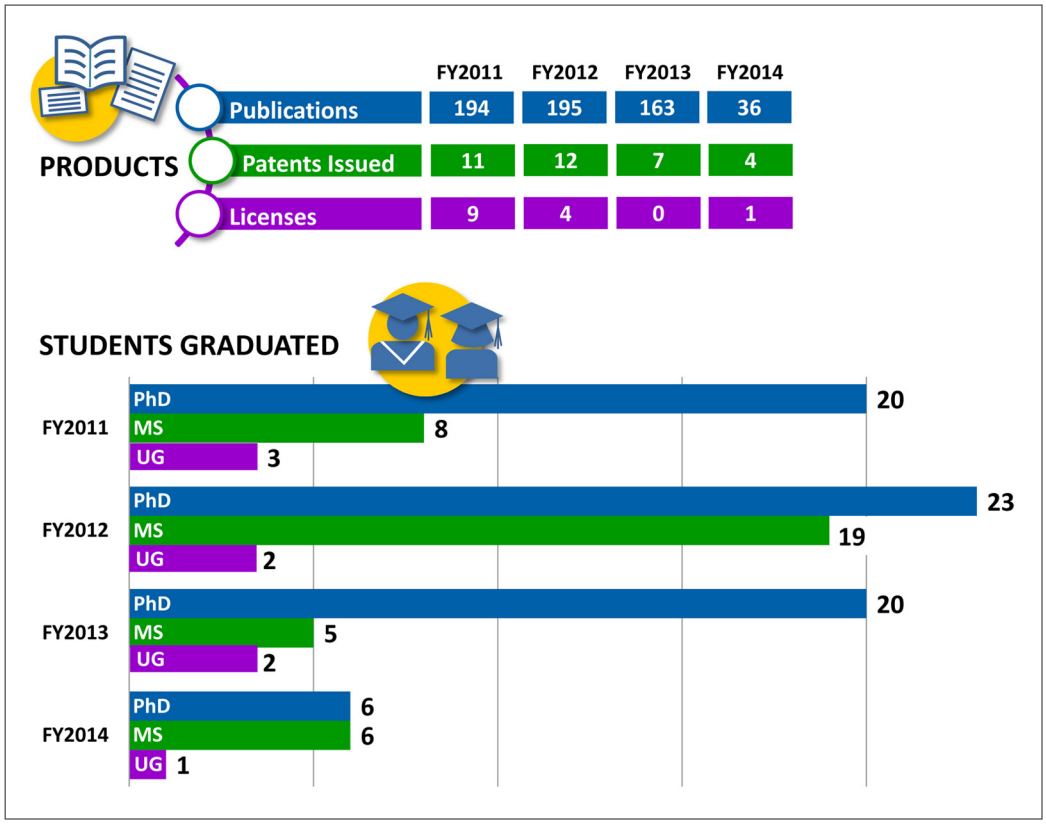
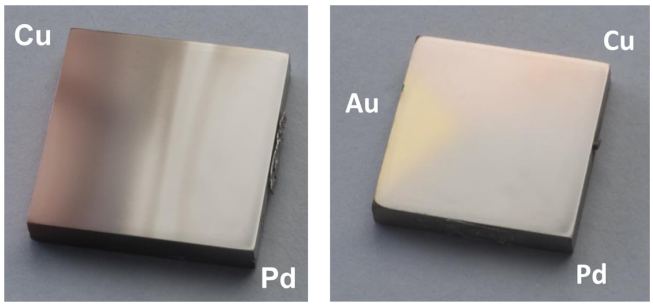


NETL Carnegie Mellon PENNSTATE University of Pittsburgh VirginiaTech WestVirginiaUniversity URS

>> **METALLIC MEMBRANES**, *Continued from Page 1*

The team—including Link, **Bret Howard**, and **Ömer Doğan**—is creating membranes with different Pd-alloy constituents in hopes of bringing the cost of the technology down while increasing separation efficiency and reducing corrosion. They have learned that the extent of corrosion depends primarily on three factors: temperature, membrane composition, and the composition and levels of corrosive contaminants in the syngas. With collaborators from Carnegie Mellon University (CMU), NETL, and industry partners, they tested gradients of Pd-alloy concentrations, which allowed them to correlate those factors with different alloy compositions. For example, they demonstrated that increasing the amount of copper (Cu) in a Pd-membrane increases its resistance to corrosion, and combining Pd with magnesium and aluminum improves corrosion resistance when the contaminants include arsenic or selenium.

Producing and delivering hydrogen from fossil fuels is a strategic national goal, and robust and cost-effective gas separation technologies will help meet that goal. The team's research takes an expensive, commonly-used membrane technology and increases hydrogen permeability while decreasing membrane degradation. These metallic membranes lead us closer to a future where hydrogen fuels are common.



Compositional Spread Alloy Films composed of gradient compositions of binary (Pd and Cu) and ternary (Pd, Cu, and gold) mixtures to test for hydrogen dissociation activity and contaminant exposure reactivity.

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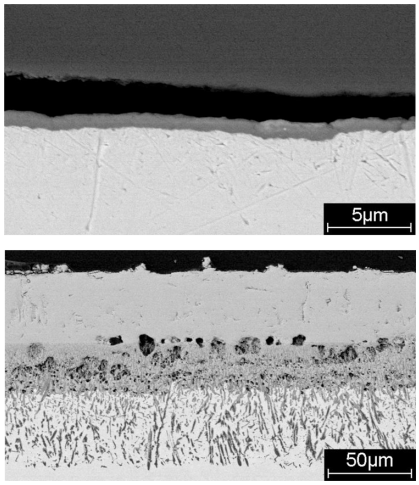
NETL-RUA Research Project Seeks to Protect Alloys in Harsh Environments

Nickel can maintain its strength at very high temperatures. It is that quality—its ruggedness—that made it the focus of an NETL-RUA research project led by NETL scientist **David Alman.** The goal of the project is to predict alloy compositions that form a protective coating (called an *oxide scale*) in a variety of environments. The project was funded by the Office of Fossil Energy, through the Cross Cutting Research Program, and it involved the work of researchers from across the NETL-RUA organization—from NETL, URS, the Pennsylvania State University, the University of Pittsburgh (Pitt), CMU, and the Oak Ridge Institute for Science and Education (ORISE) program. "It is truly a collaborative NETL-RUA effort in which data and results are exchanged between partners," says Alman. The team has already made discoveries about the diffusion of oxygen in metals that contain nickel. Those findings were reported in the *Journal of Applied Physics*.



Oxide scale formation (depicted in the upper image) protects alloys in harsh environments. Alloys that lack it (like the one shown in the lower image) are less able to withstand severe conditions.

"Diffusion is the movement of species through a medium," explains Alman. Investigating how the process is carried out in nickel alloys is worthwhile because oxygen diffusion is one of the parameters that influences how well alloys can form an oxide scale when they are exposed to high temperatures and harsh environments such as those found in advanced power systems. In particular, the team's research so far has helped them establish the computational routines necessary for predicting how even more complex alloys (such as nickel-aluminum-iron alloys) would react in particular environments (such as when they are exposed to steam or supercritical CO_2). Experimental data do not yet exist for those complex alloys, or else they are difficult to measure, says Alman. "We are currently building the computational tool set to do these predictions." That means, in the future, there may be an even wider array of alloys that can tackle crucial jobs.

Featured Facilities

No Structure Too Big, No Device Too Small: SBEUC Helps NETL-RUA Researchers Run Simulations at Various Scales

If you want to examine the properties of a structure on the nanoscale, it helps to have a powerful computer—a very, very powerful computer. So when NETL scientist **Dan Sorescu** and his research team needed to determine how single-walled carbon nanotube–titanium dioxide hybrid nanostructures interact with acetone vapors, they used NETL's Simulation-Based Engineering User Center (SBEUC), which houses the 67th most powerful supercomputer in the world.[1] The supercomputer is about a million times faster than a high-end desktop computer,[2] and it was ideal for performing their calculations.

The SBEUC's visualization center in Morgantown, WV, fosters collaborations among researchers.

The SBEUC also comes in handy when researchers need to model very large structures rather than very small ones. "I have been using the SBEUC to conduct many large-scale [computational fluid dynamics] simulations," says NETL researcher **Tingwen Li**. "For example, I ran an extremely high-resolution simulation of NETL B22 [circulating fluidized bed] riser," a task he could not have done without the SBEUC.

The SBEUC's supercomputer lets researchers "overcome the computational expense of large-scale simulations, which traditionally limited the size and scope of our modeling efforts," explains **Jordan Musser**. For his part, Musser, a researcher in NETL's Computational Science and Engineering Division, has used the SBEUC to run simulations using Multiphase Flows with Interphase eXchanges (MFIX), open-source software that NETL developed for modeling reacting multiphase flows.

Housed in Morgantown, WV, the SBEUC is fully funded by the Office of Fossil Energy, and it was designed with fossil energy research in mind. It accommodates engineering calculations that support research into fossil-fuel innovations. It also provides a way for researchers at NETL and NETL-RUA member organizations to work together as they fine-tune their inventions and predict how materials will behave in operational settings. Visualization centers at all NETL locations and collaborative workstations at each NETL-RUA member site keep researchers connected. In fact, the primary way users access the supercomputer is by logging in remotely. Advanced modeling and simulation capabilities are important to researchers, says Jordan Musser, which makes the SBEUC's many points of access especially vital.

The SBEUC's modular data center uses free-air cooling on most days of the year—supplemented by evaporative cooling on hot days—and its energy use, air temperature, and humidity are tracked.

[1]Department of Energy, *NETL's Supercomputer Addresses Energy Issues on Two Fronts*, September 26, 2013, http://energy.gov/fe/articles/netls-supercomputer-addresses-energy-issues-two-fronts, accessed March 5, 2014.

[2]National Energy Technology Laboratory, Department of Energy, *NETL Simulation-Based Engineering User Center (SBEUC)*, September 18, 2013, video, http://www.youtube.com/watch?v=HvISSd1T7fw&list=TL7GAdEhKujYTEfoHO343sU3rU0ODiq0f2, accessed February 28, 2014.

Under Pressure: ORISE Postdoctoral Researcher Works with NETL Scientists to Develop Membrane System for Carbon Dioxide Separation

It can be a challenge to separate CO_2 from a mixture of gases and prepare it for sequestration. "The major issue with capturing CO_2 from power plant flue gas is that the CO_2 makes up a small portion—13 percent—of the very large, low-pressure stream," says **Victor Kusuma**, a postdoctoral research scholar at NETL. The most widely accepted method for accomplishing the task involves using chemicals to absorb the CO_2 from the flue gas. This results in a CO_2-laden solution that is then regenerated in a steam-stripping column, which can operate only at low pressure. The steam has to be re-vaporized, and the CO_2 has to be compressed, making the process energy-intensive and costly.

The GPS column in operation.[3] The membrane system that Kusuma and the rest of the research team developed capitalizes on the GPS column's advantages for separating carbon dioxide.

To help lower these hurdles, **Scott Chen** (of Carbon Capture Scientific) invented a gas-pressurized stripping (GPS) column as part of an NETL-funded project led by NETL project manager **Andrew Jones**. The GPS column uses a high-pressure stripping gas, instead of low-pressure steam, to remove the CO_2 from the solution to be regenerated. The effluent that the GPS column emits contains a higher concentration of CO_2 than does conventional, low-pressure flue gas. Kusuma, a participant in the Department of Energy's ORISE program, collaborated with NETL research scientist **David Hopkinson** to develop a membrane separation system that exploits that property. Hopkinson is Kusuma's mentor and also part of NETL-RUA's Carbon Capture Research and Development research team.

The membrane system takes a high-pressure mixed gas feed—such as from the GPS—and separates it into two streams: a "residue" stream that has been depleted of CO_2, and a "product" stream high in CO_2. Processing the "product" stream for carbon sequestration requires less energy than processing a traditional flue gas stream. For this reason, power plants stand to reduce capital and energy costs by employing the membrane system. "We could potentially achieve a modest energy saving over the conventional stripping system," says Kusuma, "which, considering the required scale of separation, is still significant in absolute-dollar terms."

[3]Image source: Shiaoguo (Scott) Chen, http://www.netl.doe.gov/File%20Library/Research/Coal/ewr/co2/development-novel-gas-pressurized-stripping-july2012.pdf, accessed March 5, 2014.

Researchers Poised to Patent Advanced Gas Sensor

Many different streams of fuel gas now enter the nation's pipelines due to the rapid expansion of the natural gas industry. These streams, including natural gas, gasifier syngas, landfill gas, and biogas, can have radically different hydrocarbon compositions. Accurate, real-time analysis of the gas' chemical content has proven to be a critical challenge in the energy industry. Stepping in to fill the void is a team of NETL-RUA researchers working under the NETL-RUA Innovative Process Technologies Initiative.

In 1928, Indian scientist Sir C.V. Raman noted that light scatters into different wavelengths when it impinges on different molecules. Changes in wavelength can be measured, allowing the observer to draw conclusions about the chemical makeup of different materials. Today, the research team uses the distinctive emerald-green glow of a monochromatic laser to illuminate their samples and a novel sensor to collect the scattered light. They are using Sir Raman's invention to reveal the chemical makeup of fuel gases before they enter a combustion chamber. That information is critical for boosting efficiency, reducing emissions, and prolonging the life cycles of crucial equipment.

Although there are other reliable methods for sensing gaseous components, including gas chromatography and absorption spectroscopy, the NETL-RUA collaborative team's novel real-time Raman gas composition analyzer is able to quickly, accurately, and continuously monitor fuel-gas components. The team members, including **Joel Falk** and **Peng Kevin Chen** from Pitt's Swanson School of Engineering and **Michael Paul Buric** and **Stephen Woodruff** at NETL, believe that there are numerous possible uses for the sensor. Because the system provides continuous monitoring of all major fuel-gas components—reporting concentrations at better than 0.3 percent accuracy in one second or less—the sensor is used for real-time updating of natural gas compositions. One application is the continuous optimization of gas/air mixtures to increase efficiency of turbine generators.

Their patent application, titled "Gas Sensing System Employing Raman Scattering," was recently accepted by the U.S. Patent and Trademark Office. The unique sensor design provides fast, accurate, and cost-effective results and is destined for development and commercialization—falling in line with the NETL-RUA mission of technology transfer.

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