From NETL's Office of Research & Development

Research news

November 2014, Issue 2

FEATURE STORY:

Greater Than the Sum of Their Parts: Alloys for Tomorrow's Energy Systems

page 3

NETL | the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

U.S. DEPARTMENT OF ENERGY

Research news

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Dr. Geo Richards (left) discusses the lab's research with Senator Joe Manchin (forefront left) and Senator Sheldon Whitehouse (forefront right).

U.S. Senator Joe Manchin, D-W.Va. and U.S. Senator Sheldon Whitehouse, D-R.I. visited NETL on Wednesday, October 22, to see first-hand the Laboratory's cutting-edge research on advanced fossil energy technology. NETL's new director, **Dr. Grace M. Bochenek**, hosted the event that was Manchin's second visit to the Laboratory and Whitehouse's first. After referring to NETL as the U.S. "flagship of energy research," Manchin explained that he and Whitehouse were visiting each other's state to better understand the issues and challenges associated with climate change that West Virginia and Rhode Island were facing.

The two Senators met with the Laboratory's senior management team for a robust discussion about NETL's coal and oil and gas RD&D programs. They also toured several of NETL's laboratories, including the Fuel Cells Lab, Chemical Looping Reactor, and the Supercomputer and Visualization Center. There, NETL's researchers talked to the Senators about advanced research being carried out at the laboratory to improve the efficiency and environmental performance of fossil-fuel-based energy systems.

A key message conveyed to the Senators during their visit is that NETL has a proven track record for taking on tough energy challenges. Whether developing alloys for turbines to operate at higher temperatures, pioneering technologies for the recovery of shale gas, engineering systems that burn coal more efficiently, or capturing CO_2 from power plants, NETL researchers have a long history of helping to solve national and global energy issues while allowing the U.S. to continue to benefit from its domestic fossil energy resources.

Research News is a monthly publication from the National Energy Technology Laboratory's Office of Research and Development. We focus on the exciting research done at NETL by our scientists and collaborators.

Research News welcomes your comments, questions, and suggestions. Call us at **541-967-5966**.

Cover image
Dr. Paul Jablonski removes a preheated ingot from a furnace for hot working.

Greater Than the Sum of Their Parts: Alloys for Tomorrow's Energy Systems


A newly formed alloy ingot is pressed into plate form for testing.

Alloying has been used to make metals more useful ever since enterprising individuals combined copper and tin to form bronze around 2,500 BC. Since then, thousands of alloys have been created by mixing two or more elements to create new materials with more desirable qualities than any of the single elements. Carbon, for example, is added to iron to make stronger steel.

NETL houses a world-renowned alloy development research program combining expertise in computation, metallurgy, and other disciplines. Extensive research facilities allow its scientists and engineers to develop and test new alloys, from conceptualization through design of melting and manufacturing processes, to the creation of prototype components (see sidebar - page 4). Computational scientists systematically create and optimize virtual alloys, adjusting their compositions and structures in ways predicted to improve strength or corrosion resistance. Metallurgists melt and cast the most promising candidates in the laboratory—from buttons weighing a few ounces up to ingots weighing 200 kilograms—then use heat and pressure to produce sheets, plates, or rods for performance testing. Corrosion scientists and other experts join the metallurgists to evaluate the alloys' chemistry, microstructure, and performance at the conditions they will encounter in their final applications.

See a video of the creation of an alloy in the Albany NETL Fabrication Lab.

The goal is to create an alloy that can survive—and function—for tens of thousands of hours in the harsh environments so key to recovery and use of fossil fuels. Add to that challenge the fact that the conditions at which alloys must function are more severe today than they were yesterday, but less so than they will be tomorrow. Humanity, dependent on fossil fuels for centuries, has already recovered and used the most accessible coal, oil, and natural gas. We're now digging and drilling deeper to find and extract our resources, and new power generation plants must operate at higher efficiencies. Alloys for these purposes have to withstand higher temperatures, greater pressures, and more corrosive environments.

Controlling two basic alloy characteristics, chemical composition and microstructure, is crucial when creating alloys for these harsh environments. Adjusting an alloy's composition by a small amount may improve its performance so it can be used in high-efficiency plants, and composition can be manipulated to exacting requirements at NETL. **Jeff Hawk**, a senior scientist working under the Advanced Combustion program, explained, "We are able to…fine-tune the percentage by weight of the elements and improve desirable characteristics…if we need 80 to 100 [parts per million] of an element in an alloy, then we can hit that number."

For fossil fuel applications, strength at high temperature is one of the most important properties the alloy must demonstrate, and this property is largely controlled by an alloy's microstructure. When a molten alloy is poured into a mold and cooled, the size, shape, and orientation of the crystals that form (microstructure) are not constant throughout the piece of metal, nor are they arranged to give the greatest strength possible. Heat treatments cause the elements in the alloy to rearrange, changing the sizes of some

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crystals and forming new crystal phases. Forging and rolling further develop the microstructure; together, these processes dramatically improve alloy strength.

NETL scientists have patents pending for new methods to computationally design heat treatments, which will shorten the time and energy needed to achieve effective microstructures. Using these new approaches, a "recipe" is created for heat treating a particular alloy, based on its chemistry and the dimensions of the desired microstructure.

Corrosion resistance is another important performance requirement in the fossil fuel industry, where metals are exposed to hot gases, steam, and soot or ash from combustion. Under those conditions, thick layers of porous corrosion products can form and break away, leaving the metal thinner and exposing fresh surfaces to the corrosive conditions. NETL corrosion scientists investigate how to minimize destructive corrosion both in long-used and advanced alloys. With the results, "… pilot plants and larger facilities can more confidently be built and run," according to **Gordon Holcomb**, Research Materials Engineer and corrosion expert.

Industrial customers and government agencies, such as the Department of Defense, seek out NETL's unique expertise and facilities to help solve critical engineering problems related to alloy development and fabrication. NETL has developed alloys and manufacturing processes for applications as diverse as in-situ oil shale recovery, steam turbine components, rocket nozzle materials, and coronary stents. In each case, its extraordinary expertise helped achieve a unique solution. Given its history of success, NETL is up to the challenges of creating new alloys for tomorrow's energy needs and beyond.

Contact: Jeff Hawk

Titanium alloys, like the one pictured here, are commonly used in fossil energy power generation as well as the aerospace industry.

VAR/ESR Furnace and the USC Autoclave

NETL's metals manufacture and materials performance facilities comprise a full range of equipment for melting, casting, cutting, heat treating, forging, rolling, and testing metals of many types and sizes under many conditions. The two newest pieces of equipment have expanded the lab's capabilities to create and test advanced alloys for severe service environments—such as those found in fossil energy applications.

Metallurgists **Paul Jablonski** and **Joe Licavoli** use the Consarc vacuum arc remelting and electro-slag remelting (VAR/ESR) furnace to develop stringent manufacturing practices for alloy production. During electro-slag remelting, a specially designed slag absorbs and removes unwanted impurities. The VAR further refines alloy content by controlling the levels of nitrogen and oxygen in the melt with great accuracy. The large ingots created in this furnace allow NETL's research program to explore how melting practices impact the manufacture of large parts for power plants.

Other pieces of equipment test alloys at the conditions they will encounter in use, including operational temperatures of 760 °C and pressures of 5000 pounds per square inch. The ultra-supercritical (USC) autoclave was custom built for NETL, and is the first of its kind to examine how alloys react during long exposure to steam in the boilers and turbines of advanced ultra-supercritical (A-USC) power plants. Results will help predict which alloys are up to the task.

*Technician **Ed Argetsinger** lowers a cooled ingot from the vacuum arc remelting furnace.*

Novel CO_2 Capture Technology
Nets Tech Transfer Attention and National Recognition

NETL researchers have created a breakthrough technology that economically and efficiently absorbs carbon dioxide (CO_2) from fossil-fuel-burning power plant stack emissions—work that has attracted national innovation awards, as well as the attention of commercialization-minded private companies and a federal agency with plans to adapt it for space travel.

McMahan Gray, inventor and principal investigator for the project, explained that the basic immobilized amine sorbent (BIAS) technology is considered a breakthrough for two key reasons. First, it uses new high-capacity amine-based solid sorbents that maximize CO_2 removal. Second, these new sorbents can be regenerated for reuse in a novel process that reduces energy loss and minimizes moisture in the overall sorbent process, resulting in lower energy and water usage than today's wet scrubbing technology. BIAS can significantly reduce the cost penalty associated with carbon capture processes resulting in a more affordable means of generating cleaner energy from fossil fuels. Once captured, the CO_2 can be sequestered underground, or used in processes such as enhanced oil recovery.

"We tested BIAS, both at bench-scale and pilot-scale levels, and that's when it began to attract attention from the private sector," Gray explained. "At least three companies are looking at it in the [United States]."

The sorbents, which resemble pearls when viewed under a microscope, are less than 800 micrometers in diameter. By comparison, the head of a pin is about 1,000 micrometers in diameter.

BIAS could find use in other applications as well. Gray explained that the sorbent can be regenerated with a change in pressure instead of using heat. This approach makes BIAS an option for use in confined spaces—such as inside a spacecraft. "We have an interagency agreement with NASA to develop BIAS for use in space travel systems," Gray said. BIAS could be adapted as a means to purify the air inside the spacecraft.

Looking like microscopic pearls, NETL's BIAS technology enables the capture of CO_2 in large-scale processes.

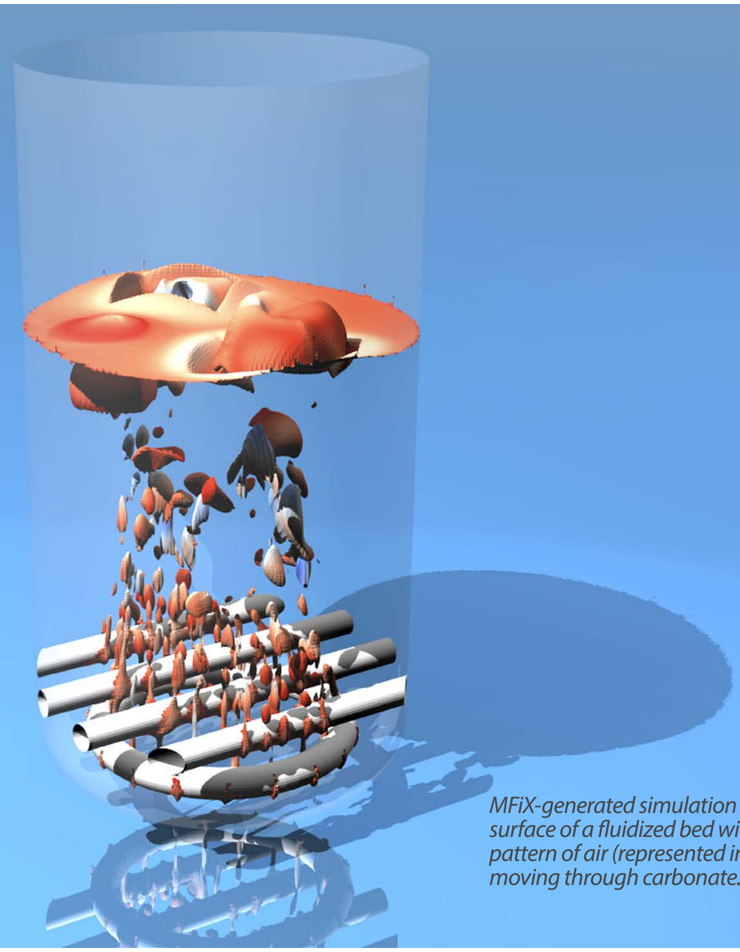
In 2012, BIAS received an R&D 100 Award from *R&D Magazine*, designating BIAS as one of the 100 most technologically significant products of the year. BIAS was also awarded the 2011 Excellence in Technology Transfer Award from the Federal Laboratory Consortium.

NETL holds two U.S. patents based on this technology: No. 8,500,854 for "Regenerable Sorbent Technique for Capturing CO_2 Using Immobilized Amine Sorbents" and No. 8,834,822 for "Regenerable Immobilized Aminosilane Sorbents for Carbon Dioxide Capture."

Contact: McMahan Gray

McMahan Gray is an inventor of NETL's BIAS technology.

Enhancing Multiphase Flow Science with **MFiX Code**



MFiX-generated simulation shows the surface of a fluidized bed with bubble pattern of air (represented in orange) moving through carbonate.

Multiphase flow is the simultaneous flow of materials of different phases (gas, liquid, or solid) or different chemical properties. It is pervasive in energy-related systems, as when coal particles interact with gases during combustion and gasification. Information from MFiX can be used to help design new fossil-fuel-driven technologies, or to efficiently assess the commercial readiness of a broad range of advanced energy technologies.

MFiX—and simulations in general—save time and money; these tools reduce the likelihood of building a piece of equipment that does not operate as designed. Engineers spend less time and money building simulations than they would building an actual structure or component.

Errors and uncertainties are inherent in any simulation, and as the complexity of the research problem grows, it becomes important to characterize them. As **Mehrdad Shahnam**, General Engineer with NETL's Multiphase Flow Team, explained, "We currently have a high level of confidence in trends resulting from simulations, but not as much in absolute values." To help define and control the uncertainties, ORD is developing uncertainty quantification (UQ) methodologies to improve the MFiX code.

Modelers from around the world are also invited to participate in NETL's Challenge Problems. This tool was created to improve the reliability of MFiX modeling of multiphase flows by validating with accurate and well-defined experimental data. Problems are described and relevant information, such as configuration of the experiment and flow conditions, is provided to the participants via the MFiX website. The participants conduct their simulations and submit the results to NETL, and NETL releases experimental results to the participants for model validation and improvement. During 2013, Small Scale Problem I addressed modeling of multiphase flows in a small-scale bubbling fluidized bed, a reactor design often used in energy and other industrial applications.

"As a modeler, you always want data for validation—the more the better—so Challenge Problems fill a crucial need for the multiphase modeling community," Shahnam said.

Model improvements that participants publish will be included in MFiX for use by the entire MFiX community. Shahnam credits NETL's university collaborations as a source of innovation and as a good way to foster long-term interest. He has observed that students who use MFiX continue to use the program when they move into research careers.

"Users have a positive experience, and so they take MFiX with them," he said. "The research community has a better tool to investigate multiphase flow, and better information here leads to more innovative technologies for energy production, which ultimately has a positive impact on the consumer."

Contact: Mehrdad Shahnam

Intern's Research Will Help Protect Drinking Water

Aubrey Harris, an intern in the Oak Ridge Institute for Science and Education (ORISE) program, became interested in hydrology when her uncle started working with Friends of the Cheat, a West Virginia–based organization that works to preserve the Cheat River watershed. That's when she discovered that engineering could be applied to solve water-quality issues.

"They were doing engineering design to use limestone to treat acid-mine drainage, but it wasn't working," recalls Harris, who is currently mentored by NETL researcher **Daniel Soeder**.

Harris was an undergraduate then, studying biological and agricultural engineering at Texas A&M University. It occurred to her that studying such topics as fate and transport of contaminants could provide her with the knowledge she needed to understand, clean up, and ultimately prevent water pollution. That has led her to pursue a master's degree in civil engineering under Leslie Hopkinson at West Virginia University (WVU), and her passion for protecting water supplies is evident in her Office of Fossil Energy–funded research.

She is investigating the sensitivity and response of field probes to surface-water properties—such as specific conductivity, pH, and dissolved oxygen—if chemicals from unconventional oil and gas development operations enter a stream. She is particularly interested in how the contaminants most frequently introduced to surface water from those activities, including produced water and drilling mud, may affect water-quality parameters. Her research focuses on chemicals that appear most often in incident reports from the Pennsylvania Department of Environmental Protection. These chemicals include ethylene glycol (a corrosion inhibitor) and polyacrylamide (a chemical, commonly called "slickwater," that is used in hydraulic fracturing).

Harris has also reviewed water-quality monitoring data generated in the wake of actual chemical spills to gain insight into which field probes are most useful for detecting specific drilling or hydraulic fracturing chemicals. Some chemicals, she explains, may be detectable with just a pH sensor. Others may need more sophisticated monitors, and her research will help to identify which probes are most effective for a given spill.

She also studies the placement of field probes to identify optimal locations for gathering valid measurements.

"I've observed several community-based groups trying to get baseline information because they knew a drill pad was being established near their reservoir," said Harris. "But, looking at their maps, you could tell the areas they were going to monitor wouldn't be affected [by the drill pad]. It's disheartening for volunteer groups to spend money on stream testing and not see anything for it."

The significance of Harris's research has not gone unnoticed. In April, a poster about her research took first place in a competition held by WVU's Davis College of Agriculture, Natural Resources, and Design. She also presented her work this year at the West Virginia Academy of Sciences meeting.

Soeder said Harris is "truly a star. She's not afraid to dive down into the weeds to do the math and the modeling to figure things out."

Results of her research will lead to an improved understanding of how energy production affects our water resources, and deliver new methods to ensure that drinking water is clean and safe for future generations.

Aubrey Harris retrieves a data logger from a stream in Morgantown, WV. (Photo by Bobby Snelson)

Mentoring Students through
Robotics Competition

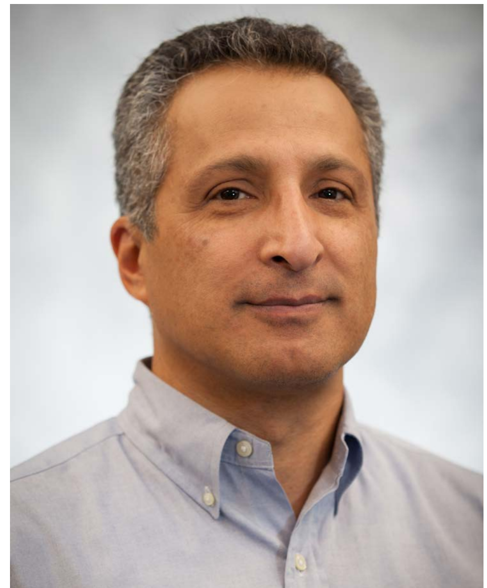
Mehrdad Shahnam, who was inspired to join NETL as a graduate student at WVU, understands the draw of fascinating science.

Shahnam's graduate project with DOE was in computational modeling and using simulations to model a sampling probe. "I learned that you can do quite a bit with computer simulations without needing to build anything," he said. "That's quite powerful and definitely fit into the 'cool' category for me."

Since then, Shahnam has dedicated his knowledge and expertise to enhancing ORD's computational multiphase flow capabilities, including NETL's open-source MFiX code. He also applies his engineering expertise as a mentor with Mountaineer Area Robotics (MARS), where he continues to witness the power of science and engineering to inspire.

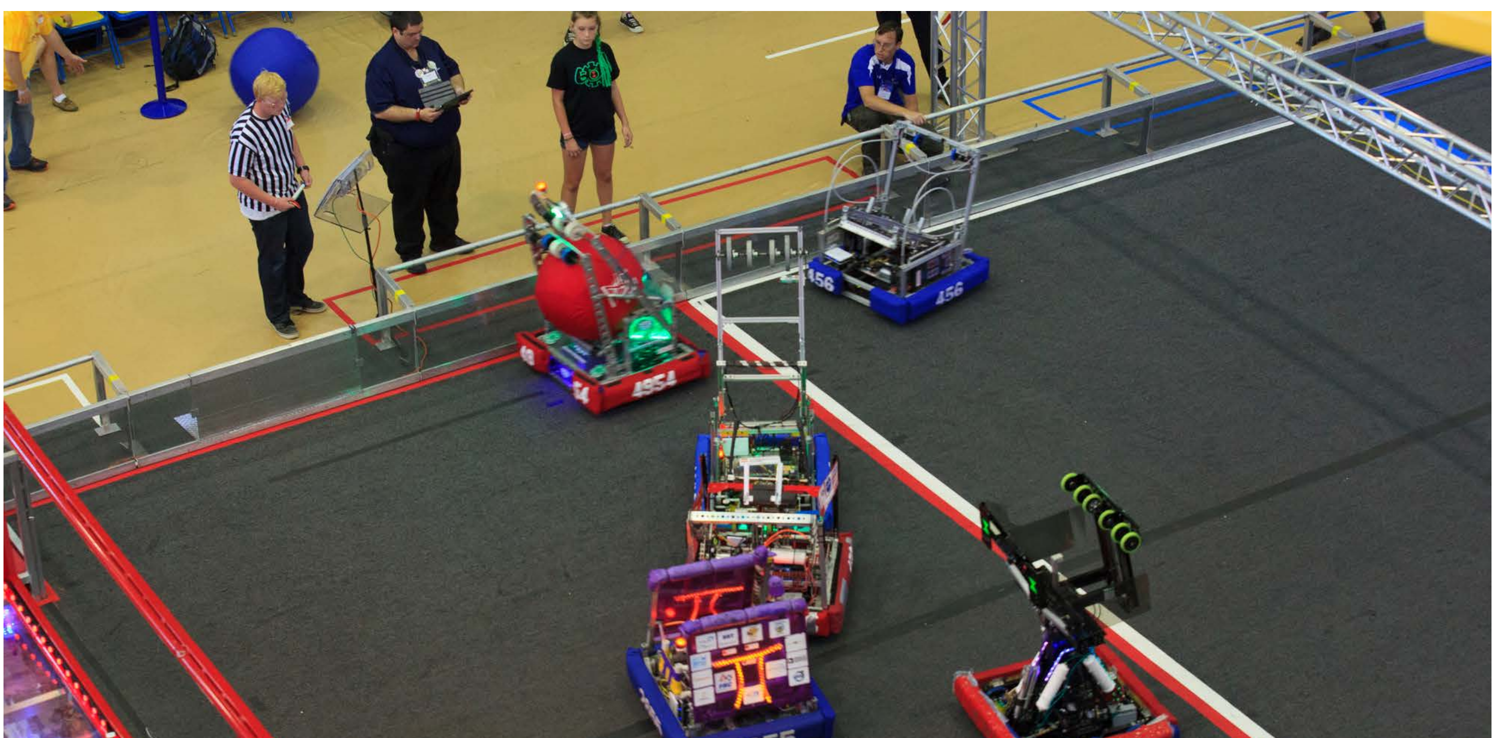
The high school MARS team that Shahnam mentors builds robots to compete in the FIRST Robotics Competition—an international event that presents students with robotics challenges and sporting events to encourage them to pursue science, engineering, technology, and mathematics fields. "Ultimately, it's a bunch of teenagers who could otherwise be doing who knows what," he said. "Instead, they come in Saturdays and Sundays to engineer, design, and work. How many teenagers would do that?" Students have 6 weeks to fabricate, program, and fine-tune the robots for competition. Shahnam says the competition is an amazing demonstration of the high school students' potential.

With the help of mentors, the students are responsible for every aspect of their robots, from conceiving the design, to fundraising, fabricating, programming, and marketing. Shahnam, whose son has been involved in robotics since he was in middle school, said the potential in young people must be nurtured.



Mehrdad Shahnam, General Engineer, Multi-Phase Flow Computation Expert

"The kids do all the work, but mentors teach them how," he explained. "They design the parts using [computer-aided design] packages and fabricate the robots. Mentors show them how to use the tools."



Students put robots through their paces at the 2014 MARS competition in Morgantown, WV

NETL's In-House Research Program:
Advanced Combustion

Advanced combustion systems promise to increase the fuel efficiency of fossil-fuel power plants and make it easier to capture—and eventually store—the CO_2 that the plants emit. One such system, chemical looping combustion (CLC), involves using a solid material, called an oxygen carrier, to deliver oxygen to a reactor's fuel. Another uses supercritical CO_2 (SC-CO_2) to drive a turbine and generate power. Gaps in technology, however, hinder the commercial deployment of these two systems. The system components are prohibitively expensive, and the materials used to operate the systems must withstand very high temperatures and pressures. To overcome these barriers, a multidisciplinary team of NETL researchers is building models and running simulations to help develop affordable, durable system components and materials. Test beds let the researchers experimentally verify the modeling and simulation results. The researchers also use a chemical looping reactor to invent and test sensors that optimize CLC system operation and autoclaves to test structural materials for the SC-CO_2 power systems. The researchers' tasks include—

- Modeling component designs and experimentally validating the models to develop more affordable, better-performing CLC components.
- Using kinetic models, computational fluid dynamics simulations, and laboratory testing to advance the performance and durability of new and existing oxygen carriers.
- Developing microwave sensors that can measure particle flow under CLC operating conditions.
- Operating experimental test beds to evaluate the performance of oxygen carriers and sensors, the operation of novel CLC equipment, the accuracy of CLC simulations and models, and the effects of contaminants on system performance.
- Carrying out laboratory- and bench-scale testing to identify and solve the problems caused by contaminants during solid-fuel CLC.
- Conducting laboratory experiments, including assessments of mechanical stability and corrosion resistance, to identify suitable materials for components of fossil-fuel SC-CO_2 power plants.

Contact: Douglas Straub (CLC); Omer Dogan (SC-CO_2 materials)

FUNDAMENTAL FUN

Alloy Basics

For thousands of years, people have been combining metals and other elements to create new materials called alloys. The dominant metal in an alloy is called the base metal, which may be any pure metal such as iron, nickel, gold, or aluminum. Other elements are then added to give the base metal improved characteristics, like strength, corrosion resistance, or thermal conductivity. Here are some interesting facts about alloys:

- Gold is usually alloyed with less-precious metals such as palladium or copper. A value called "carat weight" indicates the ratio of gold to other added metals. For example, 24-carat gold is solid gold, whereas 18-carat is only 75 percent gold.
- Not all alloys are man-made. Electrum is a naturally occurring alloy of gold and silver. It was used more than 5,000 years ago as the material for the world's first coins.
- Some alloys are not even from this planet. Meteoric iron, an alloy of iron and nickel, can only be found inside meteorites. Before mankind mastered the ability to smelt, this alloy was used to make weapons and art.
- An entire age in human history was named after an alloy. The Bronze Age occurred between 3,200 and 600 BC and is characterized by the widespread use of bronze, which is made by combining copper with tin.

*Metallographer **Paul Danielson** examines a metallic alloy at NETL*

APPLAUSE

Awards

IChemE Global Awards 2014 finalists announced:

- Young Chemical Engineer in Academia Award - **Anna Nakano** (URS)
- Energy Award - *'Foamed cement research for safer drilling'* – **Barbara Kutchko**
- Core Chemical Engineering Award - *'HTHP density measurement and EOS development'* – **Isaac Gamwo**

Book Releases

Evan Granite and **Henry Pennline** are editors of the newly released book entitled, "Mercury Control: for Coal-Derived Gas Streams." This handbook offers detailed overviews of technologies for the control of mercury, US and international regulations, and measurement methods. Published online by Wiley, available in hard copy December 2014, 480 pp.

Patents Issued

Constant Pressure High Throughput Membrane Permeation Testing System; **Erik J. Albenze** (URS); **David P. Hopkinson** (DOE/NETL); **David R. Luebke** (DOE/NETL); 8821614, issued September 2, 2014.

Electronically Conducting Metal Oxide Nanoparticles and Films for Optical Sensing Applications; **Paul R. Ohodnicki, Jr.** (DOE/NETL); **Congjun Wang** (URS); **Mark A. Andio** (ORAU/ORISE); 8836945, issued September 16, 2014.

Regenerable Immobilized Aminosilane Sorbents for Carbon Dioxide Capture Applications; **McMahan Gray** (DOE/NETL); **Sunho Choi** (GTECH); **Christopher W. Jones** (GTECH); 8834822, issued September 16, 2014.

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