Atomic layer deposition fuels future solutions to nation’s energy challenges

JENNIFER DIANJELUS

Most efficient and less costly solar cells, solid-state lighting and industrial catalysts are potential applications of atomic layer deposition (ALD), a technique that Argonne researchers are working to perfect. Other potential applications are improved superconductors and separation membranes.

ALD is a thin-film growth technique that offers the unique capability to coat complex, three-dimensional objects with precisely fitted layers. The scientists expose an object to a sequence of reactive gas pulses to apply a film coating over the object’s surface. The chemical reactions between the gases and the surface naturally terminate after the completion of a “monolayer” exactly one molecule thick. ALD can deposit a variety of materials, including oxides, nitrides, sulfides and metals.

What makes ALD more effective and flexible than traditional methods, such as evaporation, for producing thin-film coatings is its ability to coat every nook and cranny of a complex object. Scientists use this procedure to fabricate nanostructured catalytic membranes, or NCMs. These structures enable catalytic reactions that, for example, convert inexpensive feedstocks into valuable products and synthesize hydrocarbon fuels. Argonne has filed for a patent on NCMs.

“We are focusing our attention now on measuring the properties of the catalysts and synthesizing other catalytically relevant materials inside the NCMs,” said Jeffrey Elam, a research chemist in Argonne’s Energy Systems Division.

Elam, along with Michael Pellin of Argonne’s Materials Science Division, has been working with NCMs to carry out chemical reactions to produce materials that help the nation sustain itself in a more cost-effective and efficient manner.

One of the Argonne researchers’ goals has been to improve the effectiveness of the catalyst in Fischer-Tropsch synthesis. The Fischer-Tropsch process takes syngas, a mixture of carbon monoxide and hydrogen, and converts it into hydrocarbon fuels. Syngas can come from a variety of materials, including natural gas, coal or biomass.

Elam and Pellin believe that Argonne’s NCMs can improve the performance of Fischer-Tropsch catalysts enough to make the production of clean, sulfur-free fuels economically viable in the next decade or two.

Recently, Argonne researchers also have begun to apply ALD technology to solid-state lighting, which uses light-emitting diodes, or LEDs. Unlike incandescent light bulbs, LEDs consume little electric power and do not burn out or overheat. They are illuminated by the movement of electrons in a semiconductor and are considered the most efficient light source in existence. LEDs can be found in many electronic devices, from digital displays to traffic lights.

LEDs require a conducting electrode to supply electricity to the semiconducting material, but this electrode must also be transparent to allow the light to escape. Traditionally, this transparent conducting electrode is made from indium tin oxide (ITO); however, ITO is expensive.

To replace ITO, Argonne researchers are exploring chains of metal nanoparticles aligned in a magnetic field to form an electrically conductive web. ALD coatings are applied to these networks to form a transparent, conducting electrode to make cheaper LEDs. This research is funded by the U.S. Department of Energy to develop advanced solid-state lighting technologies that, compared to conventional lighting technologies, are much more energy efficient, longer lasting and cost-competitive by 2025.

In cooperation with Northwestern University, Argonne researchers are also fabricating highly efficient solar cells for converting sunlight into electricity. These improved, dye-sensitized solar cells (DSSC’s) use ALD technology in a similar way to NCMs — precisely fitted layers of transparent, conducting oxides and semiconductors deposited on the inner surfaces of nanoporous membranes.

Scientists at Argonne have started work that could provide clean, renewable fuels for transportation using a variety of feedstocks. Here, chemist Jeffrey Elam (ES), front, holds a prototype membrane that is ready to be evaluated in a catalytic testing reactor operated by chemical engineer Donald Cronauer (CMF).

The researchers aim to eventually commercialize these novel and efficient solar cells. Because no pure, costly silicon is involved in the fabrication process — as it generally is with conventional solar cells — the researchers hope to produce electricity at a much lower cost.

Felcher named inaugural fellow of Neutron Scattering Society of America

GIAN PIERO Felcher, retired senior physicist in Argonne’s Materials Science Division, has been named an inaugural fellow of the Neutron Scattering Society of America (NSSA). The NSSA selected Felcher for pioneering the development of neutron reflectometry and demonstrating its application to magnetic and polymer film systems. Neutron reflectometry involves shining parallel rays of neutrons onto a very flat surface and measuring the intensity of reflected radiation as a function of the beam angle.

Neutron reflectometry has come to be a popular way to study chemical aggregation, polymer adsorption, and (See “Felcher” on page 2)

New light cast on key chemical reactions in interstellar space

A detailed understanding of key chemical reactions that take place in interstellar space has been provided by groundbreaking research at Argonne and Sandia national laboratories and two European universities. Pictured here is the famous Orion nebula, visible with binoculars in the winter night sky.

A detailed understanding of key chemical reactions that take place in interstellar space has been provided by groundbreaking research at Argonne and Sandia national laboratories and two European universities. Argonne senior chemist Steven Klippenstein (CHM) — along with colleagues at Sandia National Laboratories; the Institute of Physics, University of Rennes, France; and the University of Cambridge, U.K. — has developed a detailed understanding of the dynamics of reactions between neutral radicals and neutral molecules, known as “neutral-neutral” reactions, at temperatures as low as 20 Kelvin, approximately the temperature of interstellar space.

In their work, Klippenstein and his collaborators determined why certain molecules reacted rapidly even at low temperatures by carefully comparing theory and experiment for a sample class of reactions (O3P + alkenes) that spans the range from non-reactive to highly reactive. The observed results from the experiment closely correlated with theoretical predictions, said Klippenstein.

“It was remarkable,” he said. “Just (See “Chemical reactions” on page 2)
The Reactions of Oxygen Atoms with Neutral-neutral reactions remain rapid throughout the whole spectrum from 20 Kelvin to room temperature. This means that we can rely on theory to predict which reactions will happen quickly. Establishing a working model for interstellar chemistry is especially important given the difficulty of performing large-scale experiments, according to Klippenstein. “My collaborators have developed some great experimental techniques for measuring these reactions at low temperatures,” he said. “But such experiments are very time-consuming and are also hard to apply to many reactions. So schemes for predicting the reactivity for arbitrary reactions, either a priori or from extrapolation, of measurements at higher temperatures are of great utility to modelers of interstellar chemistry.”

Prior experimental studies with the Reaction Kinetics in Uniform Supersonic Flow technique demonstrated that a “surprising number” of neutral-neutral reactions remain rapid at very low temperatures. As a result, such reactions can play an important role in the chemistry of interstellar space, in contrast with the conventional wisdom that interstellar chemistry is essentially all ion-based.

The paper, entitled “Understanding Reactivity at Very Low Temperatures: An experimental study in solid state physics” and a 1999 Alexander von Humboldt Foundation Research Award.

Giant magnetocaloric materials could have large impact on the environment

SYLVIA CARSON

Materials that change temperature in magnetic fields could lead to new refrigeration technologies that reduce the use of greenhouse gases, thanks to new research at the Argonne and Ames national laboratories.

Scientists carrying out X-ray experimentation at the Advanced Photon Source at Argonne — the nation’s most powerful X-ray synchrotron — are learning new information about magnetocaloric materials that have potential for environmentally friendly magnetic refrigeration systems.

Magnetic refrigeration is a clean technology that uses magnetic fields to manipulate the degree of ordering (or entropy) of electronic or nuclear magnetic dipoles in order to reduce a material’s temperature and allow the material to serve as a refrigerator. New materials for refrigeration based on gadolinium-germanium-silicon alloys display a giant magnetocaloric effect due to unusual coupling between the material’s magnetism and chemical structure.

Understanding this coupling is essential to modeling this technology from the laboratory to the household. Magnetic refrigeration does not rely on hydrofluorocarbons (HFCs) used in conventional refrigeration systems. HFCs are greenhouse gases that contribute to global climate change when they escape into the atmosphere.

A full source of X-rays for research is provided by the Advanced Photon Source at Argonne’s Advanced Photon Source Experimental Facilities. The X-rays are used to probe the magnetism of gadolinium and germanium ions as the material undergoes its bond-breaking magnetostructural transition. In addition to the expected strong magnetization of gadolinium ions, the researchers found significant magnetization attached to the germanium ions.

“This is surprising and important,” said Argonne physicist Daniel Haskel (XSD), who led the research team. “Gadolinium was expected to be non-magnetic. Its magnetization is induced by the hybridization, or mixing, of otherwise non-magnetic germanium atomic orbitals with the magnetic gadolinium orbitals. This hybridization dramatically changes at the germanium silicon bond-breaking transition, causing the destruction of magnetic ordering and leading to the giant magnetocaloric effect of these materials.”

By combining the novel experimental results with detailed numerical calculations of the electronic structure carried out at Ames Laboratory, the researchers were able to conclude that the magnetized gadolinium orbitals act as “magnetic bridges” in mediating the magnetic interactions across the distant gadolinium ions.

The magnetocaloric effect — a change in temperature accompanying a change in a material’s magnetization — is largest near a material’s intrinsic magnetic ordering temperature. In the case of rare-earth gadolinium, this occurring near room temperature and results in a temperature increase of 3.4 K per Tesla when a magnetic field is applied, making gadolinium the current material of choice for magnetic refrigeration near room temperature.

The prospects for a viable magnetic refrigeration technology recently became brighter with the report of a giant magnetocaloric effect in gadolinium-germanium-silicon-germanium alloys. The addition of non-magnetic silicon and germanium ions brings about a giant entropy change when germanium-silicon chemical bonds connecting the magnetism-carrying gadolinium ions are quickly formed or broken, respectively, by the application or removal of a magnetic field. As an added bonus, the magnetic ordering temperature can be tuned by changing the ratio or germanium to silicon.

“As a result of this work we now have a better understanding of the role of nonmagnetic elements, such as germanium, in enhancing magnetic interactions between the rare-earth metals in these materials,” said co-author and Ames Laboratory senior scientist Vitalij Pecharsky. “This discovery is counterintuitive, yet it opens up a range of exciting new opportunities towards the engineering of novel magnetic materials with predictable properties.”

Other authors in the paper are Y. Lee, B. Harmon, Y. Mudryk, and K. Gschneidner of Ames and Z. Islam, J. Lang, and G. Stajer (all XSD) at Argonne.

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RAISING DRUG-FREE KIDS TOPIC OF PHONE SEMINAR

A CQNA telephonic seminar will be held Wednesday, Aug. 8, at 1 p.m. The topic is “Raising Drug Free Kids.” To register, visit http://www.premcomft.com/webrep and use call-in number 884-8577. You must pre-register 48 hours before the start time of the seminar.

SUPERVISOR CLASS RESCHEDULED

The class “Hallmarks of Supervisory Success” has been rescheduled to Thursday, Aug. 9. The class will be held from 1-4:30 p.m. in Building 212, Room A157.

NOMINATIONS SOUGHT FOR MILLENNIUM PRIZE

The Millennium Prize Foundation, an independent fund based in Finland, is soliciting nominations for the 2008 Millennium Technology Prize. The Millennium Technology Prize is given every two years to a revolutionary invention that “promotes quality of life, contributes to the realization of human values and sustainable development.” Inaugurated in 2004, the Millennium Prize has had two recipients: Tim Berners-Lee, inventor of the World Wide Web, and Shuji Nakamura, inventor of the white light-emitting diode. The winner of the Millennium Prize receives 1,000,000 euros ($1.3 million), making it the world’s largest technology award. Nominations for the award must be received by the Millennium Prize Foundation by Oct. 1. Nominations should be sent to Cindy Willenson (CLF), Building 201, Room 258.

GUEST HOUSE COOKS UP BARBECUE WEDNESDAYS

Each Wednesday through October, the Argonne Guest House restaurant will feature a barbecue menu at both lunch and dinner.

At lunch there will be a soup and salad bar, and entrees will include barbecue ribs, chicken and fish with a cedar planked fish of the day. There will also be luncheon specials. At dinner there will also be a soup and salad bar, and entrees will include barbecue ribs, chicken, fish and steaks, as well as specials of the day. Lunch hours at the Guest House are 11 a.m.-1:30 p.m. Monday through Friday. Dinner hours are 5-9 p.m. Monday through Friday.

FEMALES SMOKERS SOUGHT FOR OSTEOPOROSIS STUDY

Women who smoke cigarettes and are four years or more past menopause are needed for an osteoporosis research study. Voluntary and sustainable, healthy. Participants will receive up to $500 compensation for blood draws, which can be carried out on-site. They will also get a free health check and complimentary gifts.

Contact information has been posted on bulletin boards throughout Argonne and is available on principal investigator Manjula H. Bhatnagarga (Ext. 32-3923 or mbhatnagra@anl.gov, or research associate Andrea Ebert-Michels (Ext. 32-3869 or aebertmc@anl.gov).

ENERGY DEPT. SEeks CANDIDATES FOR BER CHIEF, deputy FOR PROGRAMS

The U.S. Department of Energy’s Office of Science seeks highly qualified candidates to lead its Biological and Environmental Research (BER) Programs. With an annual budget of more than $550 million, the BER program is the nation’s leading program devoted to applications of biology to bio-energy technology and use and to environmental remediation.

The director of biological and environmental research is responsible for all strategic planning within the BER Program; budget formulation and execution; management of the BER office, including a federal workforce of more than 30 technical and administrative staff; program integration with other Office of Science activities and with the DOE technology offices, and interagency integration.

Further information about this position and instructions on how to apply and compose an application can be found online. Search for announcement SES-SC-HQ-014 (kd).

The deputy for programs provides scientific and management oversight of the six program offices by ensuring program activities are strategically conceived and executed; formulating and defending the Office of Science budget request; establishing policies, plans, and procedures related to the management of the program offices; ensuring the research portfolio is integrated across the program offices; establishing the DOE and program offices and other Federal agencies; and representing the organization and making commitments for the department in discussions and meetings with high-level government and private sector officials.

To apply for this position, see the announcement and application instructions online under the vacancy announcement SES-SC-HQ-014 (kd). Qualified candidates are asked to submit their online applications by Aug. 29.

http://jobsearch.usajobs.opm.gov

NEED A RIDE TO THE UNIVERSITY OF CHICAGO? A FREE SHUTTLE BUS MAKES ROUND TRIPS EVERY WORK DAY. FOR MORE INFO, SEE:

www.anl.gov/Visiting/shuttle.html

NEOS PROVIDES STATE-OF-THE-ART OPTIMIZATION SOFTWARE OVER INTERNET

Researchers at Argonne and Northwestern University have developed the Network-Enabled Optimization System (NEOS) to provide state-of-the-art mathematical optimization software over the Internet. The system has become such a success that it currently leads the field in the number of users at Department of Energy labs.

Optimization technology is essential to engineers, scientists, and businesses and even students. Optimization programs provide the answers to questions ranging from creating the most efficient allocation of resources to finding the healthiest meal at a fast food restaurant. But writing program after program to solve one optimization problem after another, or even using an existing optimization library, is often time-consuming or tedious.

“Because of its ease of use, NEOS has rapidly gained popularity,” said Jorge Moré (MCS), Argonne senior computational mathematician, who has guided the development of NEOS since its inception almost a decade ago. In 1999, fewer than 20,000 people used NEOS. In the last year alone, that number had increased to more than 225,000 users. NEOS is now the premier source of optimization technology on the Web for users of optimization software.

The popularity is due to an increased awareness that many interesting and difficult problems in science and engineering can be formulated and solved as optimization problems, coupled with the fact that more than 50 solvers are now available through the NEOS Server.

NEOS has been used extensively for a variety of applications, including modeling electricity markets, scheduling shifts for airport baggage handlers, predicting global protein folding, studying the brain’s representation system and designing low-power VLSI (very-large-scale integration systems).

Here’s how the NEOS Server works:

A user can select a program, or “solver,” for the type of optimization problem with which he or she is confronted. In order to help with the choice, an “optimization tree” provides suggestions, and each solver comes with sample problems and background information. Once the user defines the program and selects the solver, it compiles all subroutines, links with the appropriate libraries and does the necessary computations. The user is then sent the solution, along with various runtime statistics.

The latest release of NEOS provides several new features to make the server even more attractive. One new feature is the introduction of a database that enables reliable tracking of available solvers, running processes and jobs waiting to be scheduled.

“The idea came from a number of sources,” said Jason Sarich, the NEOS administrator. “We are spending less time on process management and load-balancing issues and more time on other interesting problems.”

Another new feature is the XML-RPC (Extensible Markup Language - Remote Procedure Call) interface.

“This gives users considerable flexibility in accessing the system,” said Todd Munson (MCS), an assistant computational scientist at Argonne who has been a lead developer of the vast computational infrastructure behind the NEOS Server. “Users can now easily write their own clients to access the NEOS server through a variety of programming languages,” he said.

The NEOS team consisting of Moré and three Argonne colleagues won the prestigious Beale-Oanch-Hays Prize in 2003 for excellence in computational mathematical programming. In presenting this prize, which is awarded only once every three years, the Mathematical Programming Society noted, “The NEOS Server has had a tremendous impact in the field of optimization. The influence of NEOS is such that in many applied fields the NEOS Server is synonymous with optimization.”

The NEOS Server is maintained under the aegis of the Optimization Technology Center, a joint project of Argonne and Northwestern University, and is operated with support from the Mathematical, Information and Computational Sciences Division of the Office of Advanced Scientific Computing Research in the U.S. Department of Energy’s Office of Science.

SERVICE AWARDS FOR AUGUST

45 YEARS

James E. Emerson (ERM)

40 YEARS

Victor A. Maroni (CMT)

35 YEARS

Michael P. Deyar (FMS), Elisa M. Mackay (CIS), Darinka K. Mones (NE), Derrick Yeager (FMS)

30 YEARS

Barbara L. Canturos (DIK), Kathleen S. Rank (ES), Darinka M. Voss (AST)

25 YEARS

Terry L. Carbaugh (FMS), Carol J. Reaves (OCF), Richard G. Black (CIS), Dawi Tave (CIS)

20 YEARS

Uthamalingam Balachandran (MS), Mathai Batmaz (FMS), Patricia C. Combis (SCC), Thomas E. Hallman (FMS), Daniel J. McManis (NOD), James G. Parker (OCF), John E. Pearson (MSD), Philip C. Rash (FMS), Juan R. Ribbns (CIS), Mary Ann Widing (DII)

15 YEARS

Jeffery Altz (FMS), Dale C. Baucom (FMS), William G. Janzarik (AIS), David Lichty (ASD), Joseph Mai (ISD), Emil Trabeniak (AES), Leszogido Villasam (FMS)

10 YEARS

John J. Amn (EVs), Man E. Middendorf (ASD)

5 YEARS

Edward A. Hoffman (NE), Roderick Matamala Panadel (BIOS), Leonida E. Ocola (CHMI), Richard Soto (SCI), Jeffrey John Ullian (EOC), Stefan Vajda (CHM)

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Argonne “...for a brighter future”
Horses won the top honors in the men's division. The grand prize winner of Argonne Combined Appeal's annual raffle was Karl Duke (OCF), who won two United Airlines tickets to anywhere in the continental United States.

Uncle Bub's Barbeque of Westmont was the food vendor for the event. The Argonne Club provided free snowcones, popcorn, cotton candy, etc.

“Overall, the picnic was a great success. A special thanks to all our volunteers — we could not put on this event without them,” said Stepuszek.

All photos by George Joch.