Turning Sodium-Tungsten-Bronze into Tungsten Carbide Needles

Carlos Bamberger, a chemist at Oak Ridge National Laboratory, has discovered a chemical method for producing tungsten-carbide needles from needle-shaped crystals of sodium-tungsten-bronze, an inexpensive material. The chemical reaction used is a "pseudomorphic reaction" in which the final product has the same shape as the material initially used in the reaction. Bamberger expects this knowledge to be applied to the development of ceramic needles that could be added to metal to strengthen it for use in engine parts.

"The performance of a material is often strongly dependent on its shape, or morphology," Bamberger said. "Because the morphology of a material during manufacture cannot be predicted, this work is valuable because it shows for the first time that needles of tungsten carbide can be made from needles of another starting material."

To produce a material that is about 75–80% tungsten carbide and about 20–25% tungsten metal, Bamberger reacted solid crystals of sodium-tungsten-bronze with various hydrocarbon gases at high temperatures. He altered the proportions of tungsten carbide and tungsten metal by varying the temperature, flow rate, and composition of the hydrocarbon gas.

Bamberger said that properly shaped tungsten carbide could be used to form ceramic composites and ceramic-metal composites that have industrial use.

Thousands of Metal-Oxide Compounds Tested at Once

Researchers at the Ernest Orlando Lawrence Berkeley National Laboratory's Molecular Design Institute have found a way to deposit thousands of distinct combinations of metal-oxide molecules onto an area the size of a checkerboard square, thereby creating the first "combinatorial" library of advanced materials.

The combinatorial strategy is a departure from so-called rational design, where researchers try to predict beforehand which molecular structures will yield desired properties. The new strategy relies more on sheer numbers—making a myriad of theoretical candidates and sorting through the bunch to find a solution.

The technique uses masks to stencil thin layers of metal-oxide ingredients onto different columns and rows of an inch-square grid. The technique has been used to create libraries of high-temperature superconductors. Metal components are laid down atop one another, each layer 10 to 100 Å in thickness. The layers are heated to mix the metal elements and create a stable, composite compound.

The researchers create arrangements of different metal combinations by depositing the thin films through masks. A so-called primary mask is used to lay the metals down as a grid of separate squares. A secondary mask, when laid atop the primary mask, serves to block out specific rows or columns of the grid. By sending the metals through different secondary masks, each can be deposited on particular sections of the grid.

To test the technique, the researchers first created a small, 16-member library of copper-oxide high-temperature superconductors. The researchers laid down a base layer of copper through the primary mask then deposited layers of oxides of bismuth, calcium, lead, and strontium through different secondary masks. Because of the sequence of masks, each site on the grid received a different combination of metal oxides and each combination was represented once.

After heat treatment, the researchers tested the electrical characteristics of the materials in their library. Results showed the copper-oxide thin films had the same resistive characteristics as superconductors created by large-scale means. The researchers then made denser, 128-site superconductor libraries with combinations of seven metals.

Tests with decreasing mask sizes showed that the method could produce working superconductor films as small as $200 \times 200\ \mu m^2$. At scales below 200 μm, metal-oxide molecules in the thin layers began to evaporate.

"With 200-micron sites, we can realistically deposit 10,000 materials in a square inch area," chemist Peter Schultz said. "That would effectively increase the rate at which we can test new materials by a factor of 10,000."

The research was described in Schultz and physicist Xiao-Dong Xiang's article in the June 23 issue of the journal *Science*.

Recently Announced CRADAs

Advanced Refractory Technologies, Inc. (ART) (Buffalo, New York) and **Phillips Laboratory** (Albuquerque, New Mexico) signed a one-year CRADA agreement for $250,000 to test and evaluate ART's thin film coating technology for field emission performance and stability in field emission cold cathodes for use in high power microwave devices.

Molecular Magnets Attract Interest

Gregory Girolami of the Materials Research Laboratory at the University of Illinois at Urbana-Champaign has developed a method to prepare "molecular magnets," which are materials systematically magnetized at a molecular level. The researchers made the magnets by linking small inorganic molecules into three-dimensional materials in which the molecular structure guarantees its magnetism. These molecular magnets can be made at room temperature, and they remain magnetic at temperatures well above 30 K, the temperature at which most other "molecular magnets" lose their magnetic properties.

Most magnets are ceramic or alloys, and have to be prepared at very high temperatures, often above 1000°C. The process can be costly and energy-consuming. The goal of Girolami's research was to determine how to modify molecular structures to obtain materials with relatively high magnetic ordering temperatures. The next step in his research is to develop a general route to molecular magnets that remain magnetic above room temperature.

Seraphim Train Empowered by Magnetic Coils

Scientists at Sandia National Laboratories have developed a concept for a high-speed, magnetically powered train that does not levitate, is relatively inexpensive to build, and can run on already-laid track.

The working model consists of a vertical, two-foot tall aluminum plate that slides along a rail, is powered by magnetic coils, and in 12 feet reaches a speed of 34 mph.

The proposed train would carry its own drive mechanism of a gas turbine that powers on-board electromagnets. The pulsed magnets induce reversed electric currents in a series of aluminum plates bolted to or near the track. The induced currents create their own magnetic fields that oppose those of the train. With the aid of optical sensors, the fields pulse on just as the magnets pass the midpoint of the aluminum plates, and by repulsion propel the train forward.

This magnetic field that repels the train, enabling the train to achieve high speeds, is the basis for the acronym that forms its name: Segmented Rail Phased Induction Motor (Seraphim).

The train is expected to travel at 200 mph. The current maximum for commuters on the corridor between Boston and Washington is 100 mph.

Computer Modeling Assists Scientists in Creating Nanomachines

Scientists in Oak Ridge National Laboratory's (ORNL) Chemical and Analytical Sciences Division are focusing on building machines at the atomic level.

"Over the past 15 years, prominent scientists like Noble Laureate Richard Feynman, Eric Drexler and Ralph Merkle have hypothesized about these mechanical machines," said Don Noid, one of the originators of the project. "Now, ORNL is modeling nanomachines using fundamental calculations."

Noid and colleagues Bobby Sumpter and Robert Tuzun perform these calculations using computational chemistry and other advanced visualization techniques provided by Ross Toedte of ORNL's Center for Computational Sciences. Essentially, Toedte "makes movies based on our calculations about how these machines would perform," Noid said.

Using computer modeling, the researchers simulated how fluids flow through nanomachines. They also designed a simple graphite bearing and shaft composed of about 4,000 atoms. By studying these models, researchers hope to demonstrate that they can eventually build nanomachines.

"Machines start with simple components such as rods and bearings," Sumpter said. "We would like to investigate through computer modeling and simulation whether primitive components—atomic-scale gears and bearings—could be made and successfully used to perform useful functions."

Magneto-Optical-Flux Imaging Locates Interruptions in Electric Flow

A joint research project conducted by Phase Metrics of San Diego, Argonne National Laboratory in Illinois, and scientists from the Institute of Solid State Physics (ISSP) outside Moscow produced an imaging technique that could lead to improved magnetic materials such as for recording devices and floppy disks.

The research project uses magneto-optical-flux imaging to pinpoint the tiny particles that interrupt current flow in high-temperature superconductors. Key to the process is a special indicator film invented by the researchers at ISSP.

Now that researchers can image the roadblocks to current flow, they can experiment with different superconducting samples to make the best pathway for the electrical current, said Carlos A. Duran of Phase Metrics. The imaging technique is already being used to improve the performance of commercial wires in a joint Argonne-industry program sponsored by the Department of Energy. The technique is the subject of an article in the July 6 issue of the scientific journal *Nature.*

New Route for Methane Activation Discovered

In research conducted at the University of Pittsburgh's Surface Science Center, Jason Wong, Todd Ballinger, and John T. Yates, Jr. have discovered a type of heterogeneous process that can activate the C-H bonds in methane and other hydrocarbons, which will help convert this molecule into useful organic products.

The reaction center is the well-studied $Rh(I)(CO)_2$ species, which is bound on the

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oxide support surface. Methane activation is initiated when a CO ligand is photolytically desorbed by uv radiation to produce the Rh(I)(CO) surface species. Rh(I)(CO) presents a coordinatively unsaturated Rh site, capable of interacting chemically with methane or other saturated hydrocarbons containing C-H bonds.

This unsaturated surface site has been shown to break C-H bonds in hydrocarbons, causing surface species such as Rh(III)(CO)H(CH_3) to be formed. Then the CH_3 group inserts itself into the remaining Rh-CO bond, making an acetyl species, CH_3CO, which is also bound to the Rh center. This discovery provides a potential heterogeneous route to useful organic products.

Since the use of uv light to initiate this type of chemical reactivity would be expensive, the researchers are working on finding a "thermal window" where the coordinatively unsaturated site, with its strong reactivity, can be produced using heat alone.

The photochemically initiated reactions discovered on the heterogeneous catalyst have their analogs in the homogeneous coordination chemistry of Rh compounds, and the idea to look on surfaces for this type of reactivity originated from homogeneous phase photochemical studies being done, for example, by Robert G. Bergman and his group at the University of California—Berkeley.

Coal Pollution Converted into Sulfur

Researchers at Oak Ridge National Laboratory (ORNL) have developed a technique to convert sulfur dioxide—a pollutant from coal-fired steam plants that causes acid rain—into sulfur.

Eric Kaufman, a researcher at the Bioprocessing Research and Development Center in ORNL's Chemical Technology Division, and P. T. Selvaraj, a postdoctoral scientist at the center, introduced into a vertical glass cylinder, or bioreactor, two types of bacteria-sulfate-reducing bacteria (SRBs), which cannot tolerate oxygen, and heterotrophs, which remove oxygen to help the SRBs survive. The bacteria are fed a sewage digest that provides them with carbon, their main food source.

In the bioreactor, gelatinlike beads containing SRBs are suspended in sewage media through which sulfur dioxide flows. The SRBs convert the sulfur dioxide into hydrogen sulfide, which can be chemically or biologically converted to elemental sulfur.

Sulfur is used to make chemical-sulfuric

SBIR Update

Eltron Research, Inc. (Boulder, Colorado) received a Phase II SBIR award from the Department of Energy to develop Eltron Ceramic Membrane Reactor (CMR) technology for synthesis gas production. The approach will use heat generated by the exothermic methane partial oxidation reaction to drive the endothermic steam reforming reaction.

Molecular Simulations, Inc. (Burlington, Massachusetts) will use a Phase I SBIR grant from the National Institutes of Health to develop three-dimensional structure libraries for use in combinatorial chemistry.

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acid, which is essential to the manufacture of plastics, fertilizers, and other products.

Selvaraj is developing another bioreactor process for converting the hydrogen sulfide to sulfur. This process will use sulfur-oxidizing bacteria, which add oxygen to hydrogen sulfide, producing water and sulfur.

Treated Glass Fibers Reduce Contaminants in Air, Water

Scientists at the University of Illinois at Urbana-Champaign have developed a low-cost, highly versatile separation system that can remove trace contaminants from air or water to concentrations far below the level achievable using current processes. The system works by controlling the chemistry of activated phenolic resins coated onto glass fibers and manipulating pore size.

Experiments have shown that a wide variety of contaminants can be reduced to the range of parts per billion, far below levels attainable by using conventional activated carbon granules, according to principal investigator James Economy, head of the Department of Materials Science and Engineering, and doctoral students Chris Mangun and Mike Daley.

An advantage of the fibrous form over granules is the ability to provide better contact with the medium, and to filter out particulates down to submicron range, Mangun said.

In model experiments involving p-nitrophenol, which is on the Environmental Protection Agency's list of priority toxic pollutants in water, Mangun reduced an initial concentration of 15 parts per million to less than 1 part per billion by modifying the pore surface chemistry of the adsorbent. The adsorbent can be regenerated *in situ* by electrical resistance heating.

Morris Cohen Receives Acta Metallurgica J. Herbert Hollomon Award

The sixth annual Acta Metallurgica J. Herbert Hollomon Award has been awarded to Morris Cohen, Institute Professor Emeritus at Massachusetts Institute of Technology. The award recognizes outstanding contributions to understanding the relations between materials technology and society, and/or contributions to materials technology and society, and/or contributions to materials technology that have had major impact on society. Cohen was selected for the award in recognition of his leadership in guiding U.S. national materials policy and the evolution of the multidiscipline of materials science and engineering, as well as for his teaching and research contributions.

Cohen's research has played a seminal role in understanding the mechanism and kinetics of martensitic and bainitic phase transformations, measurement and theory of nucleation in displacive transformations, tempering phenomena and strengthening mechanisms in martensitic steels, solid-state thermodynamics, deformation-enhanced diffusion, deformation-induced transformations and transformation plasticity, structure-property relationships in microalloyed steels, and rapid solidification of crystalline alloys. □

Aaron N. Bloch, provost of the State University of New York at Buffalo, died unexpectedly on April 8, 1995 in his East Amherst home. He was 53.

Bloch held a BS degree in chemistry from Yale University and a PhD degree in chemical physics from the University of Chicago.

He was a postdoctoral research associate at the Massachusetts Institute of Technology before joining the faculty of Johns Hopkins University in 1969, becoming full professor in 1977. In 1980, he left Johns Hopkins for a senior scientific position with the Exxon Research and Engineering Co. He was named director of its Physical Science Laboratory in 1984.

He left Exxon to become a vice provost of Columbia University. After four years at Columbia, Bloch accepted the provost position at SUNY at Buffalo.

He was a member of the Public Affairs Committee of the Materials Research Society and had been active in the Society's council and various committees, including the External Affairs and Long Range Planning Committees.

Aaron Bloch worked tirelessly to improve the educational environment of his home insititution and the nation in general. He will be sorely missed by his many colleagues and friends.

Gerhard Ondracek, materials science chair and director of Technisches Institut: Materialwissenschaft at Friedrich-Schiller-Universität Jena, died in a car accident in Germany on May 22, 1995. He was 60 years old.

Werner Lutze of the University of Mexico said, "We are losing an expert in materials science who was full of excellent ideas and who had just started to bring a major thrust to the field of new materials through recycling."

Ondracek received his masters degree from Technische Hochschule Magdeburg and his PhD degree from Stuttgart University. He was a research scientist at the Kernforschungszentrum Karlsruhe for over 20 years and associate professor of materials science at Karlsruhe University. During 1982 to 1986 he was a research fellow in international mission in Argentina and Brazil. During 1987–1992, he was full professor and head of Institut für Gesteinshuettenkunde at Rheinisch-Westfälische Technische Hochschule Aachen. He was a visiting professor at Technische Universität Wien in 1993 and joined Friedrich-Schiller-Universität in 1994.

Ondracek was the new Principal Editor in Europe for the *Journal of Materials Research*, published by the Materials Research Society. Ondracek had also volunteered in the preliminary planning for potential 1996 MRS Fall Meeting symposia.

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