

of *Electrochemical and Solid-State Letters* by collaborators at National Chiao-Tung University and National Nano Device Labs, Taiwan, and University of Illinois at Urbana-Champaign. This metal-oxide dielectric was formed using direct oxidation of sputtered Co/Ti films.

Samples were fabricated on *p*-type (100)-oriented silicon wafers. First, an ultrathin, ~10 Å-buffered layer of either Si-N or Si<sub>3</sub>N<sub>4</sub> was formed to improve the interfacial quality. The former was created by growing a nitrided oxide on silicon, while the latter by NH<sub>3</sub>-nitridization. Afterwards, the 50-Å Ti and Co films were deposited using the sputtering method, then direct thermal oxidation was conducted at 700 or 800°C in diluted O<sub>2</sub> gas, and annealed in N<sub>2</sub> gas ambient. Finally, a gate electrode of aluminum film was deposited on the wafer by a thermal coater.

X-ray diffraction analysis shows that NH<sub>3</sub>-nitridization can suppress the diffusion of the metal, resulting in a pure CoTiO<sub>3</sub> phase, as also exhibited by transmission electron microscope cross-sectional analysis. The effective dielectric constant of CoTiO<sub>3</sub> gate dielectric film was proposed to be about 40. A smooth interface between the nitride and silicon substrate also suggests a good interface quality. CoTiO<sub>3</sub> samples buffered using Si<sub>3</sub>N<sub>4</sub> show a lower leakage at low field and a higher breakdown voltage than those of Ta<sub>2</sub>O<sub>5</sub> or TiO<sub>2</sub>. It also demonstrates a high reliability after 10<sup>4</sup> s stressing.

WIRAWAN PURWANTO

### Au, Ag, and Pt Nanowires Produced in Mesoporous Silica

Metal nanowires with tunable diameters below 10 nm have been intensively studied because they provide an excellent platform for investigation of the fundamental physics of nanowires and have potential applications in electro-optic chip devices. Professor Galen D. Stucky, postdoctoral associate Ji Man Kim, and graduate student Yong-Jin Han at the Department of Chemistry and Biochemistry at the University of California—Santa Barbara have introduced a method for the synthesis of such nanowires. The researchers produced Au, Ag, and Pt nanowires by reduction of the corresponding metal salts loaded into the pores of the mesoporous silicate template SBA-15. SBA-15 is characterized by large surface area; variable pore diameter (4–30 nm); a well-ordered, hexagonal array of pores; and long-range order. The resulting nanowires were 7 nm in diameter and 50 nm–1 μm in length. Free nanowires produced by dissolution of the template had an average length of 0.5 μm and retained the 7 nm diameter.

As reported in the August issue of *Chemistry of Materials*, SBA-15 with 7 nm diameter pores was loaded with precursors by immersion in an appropriate aqueous salt solution followed by drying and treatment with methylene chloride to force the outer surface bound precursors into the channels of the SBA-15. The loaded template was then dried in a vacuum oven, and the Au, Ag, and Pt salts reduced under continuous hydrogen flow at 393, 623, and 593 K, respectively. The SBA-15 was dissolved with HF/H<sub>2</sub>O/ethanol to obtain free nanowires. Longer nanowires can be obtained by varying the degree of template loading and the annealing temperature. Thicker nanowires can be prepared by using SBA-15 with a larger pore diameter.

The researchers said that x-ray diffraction studies of the metal/SBA-15 samples demonstrate the formation of reduced metals with a 2D hexagonal structure and excellent textural uniformity. The pres-

ence of reduced metal in the template was confirmed by energy dispersive x-ray measurements. The dimensions of the nanowires were obtained from transmission electron micrographs.

According to Stucky, mesoporous silicates like SBA-15 are ideal candidates for templating nanostructured phases because they are durable, highly processable, and easily interfaced with silicon wafers to create nanostructured optical waveguides, chemical sensors, optical switches, and microlasers. The Stucky group is currently working on the synthesis of various nanostructures in a number of mesoporous silicates.

GREG KHITROV

### Software Package Performs Molecular Dynamics Simulation with Over 5 Billion Particles

Using a recent upgrade of the Cray T3E-1200 at the Jülich Supercomputing Center,



W. David Kingery, Professor of Materials and Archaeology at the University of Arizona, passed away on June 30 at his home in Wickford, Rhode Island, at age 73. He was an ex-MIT professor and long-time resident of the Boston area who became known as the “father of modern ceramics” for his role in providing a scientific foundation to the empirical practice used since ancient times to manufacture pottery, chinaware, tile, brick, cement, and glass. He received a SB degree in chemistry (1948) and ScD degree in ceramics (1950) from MIT, and served on the MIT faculty in

the Department of Materials Science and Engineering from 1951–1988, where he was the first to hold the Kyocera Professorship. In 1988, he joined the University of Arizona to pursue interdisciplinary studies between Materials Science and Archaeology. In 1992 he was honored with the title of Regents Professor, the highest rank in the Arizona system. In the early 1950s, Kingery established at MIT the first graduate education and research program in the science and technology of ceramics, and wrote in 1960 the first edition of a seminal textbook *Introduction to Ceramics*, now in print for 40 years and translated into the world’s major languages. His scientific research led to the development of advanced materials with unique electrical, thermal, mechanical, and chemical properties. Ceramics are used today in technologies such as automotive oxygen sensors, fuel cells, and a vast range of electronic components. In 1999, he was awarded the Kyoto Prize by The Inamori Foundation of Kyoto, Japan, for systematically integrating the knowledge and practice related to ceramic materials into a scientific discipline. Accompanied by his wife, Dr. Kingery is shown in the photo receiving the Kyoto Prize. In recent years, Dr. Kingery also analyzed, from an archaeological standpoint, the earthenware, pottery, and chinaware that are found throughout the world—studying the development and diffusion of ceramic techniques and providing cultural and anthropological interpretations of advanced technology. Dr. Kingery was interested in exploring how specific case studies related to “the big picture”—the broader issues of technology transfer, technological change, producer and consumer roles in design, technology, and engineering education. His recent books—*History from Things* (S. Lubar and W.D. Kingery, eds., The Smithsonian Press, Washington, DC, 1993) and *Learning from Things* (W.D. Kingery, ed., The Smithsonian Press, Washington, DC, 1996)—reflect these interests. Among his other recent books are *Japanese/American Technological Innovation* (W.D. Kingery, ed., Prentice Hall, Englewood Cliffs, NJ, 1991), and *Physical Ceramics* (Y.-M. Chiang, D. Birnie III, and W. D. Kingery, John Wiley and Sons, NY, 1998).

Dr. Kingery was also an avid sailor who co-organized the Marion-Bermuda Cruising Yacht Race, first sailed 20 years ago, which continues to this day. He is survived by his wife Lily (Koers); a son, William of Rolling Hills, Va.; a daughter, Rebecca Jones of Burlington, Mass.; a stepson, Bart H. LaPoole of Norwalk, Conn.; a stepdaughter, Marina Vooren of Wichita Falls, Texas; two brothers, John M. of Greenwich, Conn., and Robert E. of Charlotte, NC; and nine grandchildren.

DUNBAR P. BIRNIE, III

a group at the Institut für Theoretische und Angewandte Physik (ITAP) of Stuttgart University carried out a demonstration run with over five billion particles. With 512 processing nodes and a total memory of 256 GB, the program IMD (ITAP Molecular Dynamics) performed a simulation with 5,180,116,000 particles.

The atoms, interacting via Lennard-Jones potentials, were placed in a cubic fcc lattice cell with an edge length of 1540 atom distances or 0.42  $\mu\text{m}$  (for Al). This means that the simulations are arriving at scales comparable to the wavelength of visible light and to the width of the conductor paths of the computer. Six time steps were carried out and took a computer time of 2,328 s. According to the researchers, 223 time steps would require about a day, a typical simulation more than a month. The real challenge, they said, is the output data which cannot be stored directly but has to be analyzed parallel to the simulation.

IMD is a software package designed to perform classical molecular dynamics simulations on massively parallel computers. The interactions are not limited to pair potentials. The program permits embedded atom potentials, three-body potentials, and anisotropic Gay-Berne-potentials. In addition to the common thermodynamic ensembles, a number of boundary conditions are implemented enabling the program to deform a sample, to stress load it, or to simulate shock waves.

### AFM Applied in Molecular-Scale Flattening of DAST Crystals

Due to their nonlinear optical properties, certain organic crystals are useful in applications such as ultrahigh-speed signal detection and integrated circuit diagnosis. While the polishing of these soft organic crystals is required for optimizing light transmittance, the usual polishing and cutting techniques are often insufficient for flattening these materials. A research group from the Institute for Chemical Reaction Science at Tohoku University and the Intelligent Cosmos Research Institute has invented a molecular-scale polishing method utilizing atomic-force microscopy (AFM). As reported in the August 1 issue of *Optics Letters*, ion pairs of the 4-dimethylamino-N-methyl-4-stilbazolium tosylate (DAST) crystal may be removed by applying some force to the AFM cantilever tip.

Single DAST crystals were grown from seed crystals by lowering the temperature of a solution saturated with DAST. The flattening of the (001) surface was performed by the scanning action of the AFM. "When the force applied to an AFM tip is larger than that of the interlayer bond, the

layer(s) that are exposed on the surface will be removed," the scientists reported. An approximately 10 nN force was applied to the tip (with a tip curvature of 20 nm) during the scan. Three stepped terraces appeared after the first five scans, and another five after eight scans. The average step height was approximately 0.9 nm. This is a good agreement with the interlayer distance of 0.893 nm. The scientists generated a terrace area of 250,000  $\text{nm}^2$ . A few existing terrace steps are not expected to contribute significantly to optical transmission loss.

A friction-force microscope (FFM) was used for characterizing the resulting DAST crystal. Topography photos indicate that terrace regions are indeed very flat, with a roughness of 0.12 nm rms. These results show that the AFM may be used as a polishing tool and that this technique shows promise for other organic crystals similar to DAST.

JUNE LAU

### Minimization of Diffuse Scattering Reduces Resistivity of Thin Copper Films

Low resistivity values of 2–2.2  $\mu\Omega\text{ cm}$  have been observed for copper films as thin as 30–40 nm, comparable to the mean free path (mfp) of electrons in copper. A team of researchers at Rensselaer Polytechnic Institute (RPI) reports that the deposition of copper thin films in an argon atmosphere containing 3 vol% hydrogen followed by a low temperature anneal considerably improves the conductivity of the films.

As semiconductor devices continue to shrink, the dimensions of the interconnect metals reach values comparable to the mfp of electrons. This results in a drastic increase in resistivity, which is attributed to diffuse electron scattering by surfaces. Passivation or tailoring of the surfaces that results in an increase of the elastic scattering component should therefore decrease the resistivity.

"Our experiments were designed to find conditions that may lead to a passivation of surfaces and thereby decrease the resistivity of thin copper films (30–50 nm). Earlier studies by Ficalora have indicated that sputter-depositing Cu in hydrogen lowered the as-deposited resistivity of Cu films that were greater than 100 nm in thickness. Ficalora has also shown that electromigration testing in hydrogen ambients caused significant improvements in the electromigration lifetimes of Au interconnects," said S.P. Murarka, professor of materials science and engineering at RPI.

As reported in the September issue of

*Electrochemical and Solid-State Letters*, the scientists investigated films between 10 and 200 nm in thickness prepared by dc magnetron sputter deposition of copper. Substrates were *p*-type silicon with a uniform 50 nm thermally oxidized layer. The copper depositions were carried out in pure argon or in argon with 3 vol% hydrogen and annealed in high vacuum or in an argon atmosphere with 3% hydrogen at 300°C. The films that were prepared in the hydrogen-containing atmosphere showed a resistivity that was on average 10% lower than for films prepared in pure argon, and the resistivity at 39 nm thickness was estimated to be 2–2.2  $\mu\Omega\text{ cm}$ . The resistivity of the films deposited in pure argon could be decreased by 10–30% by annealing in vacuum or Ar/H<sub>2</sub>. The use of Ar/H<sub>2</sub> gave 2–5% lower resistivity values than the vacuum treatment.

"The role of hydrogen in affecting the resistivity of as-deposited films is not clear yet," said Anupama Mallikarjunan, a graduate student in Murarka's group. "It seems to passivate the electron-scattering defects including surfaces, enhancing the overall mobility across the film."

Another factor, according to the researchers, could be that hydrogen scavenges the chamber of impurities like oxygen, water, and nitrogen. Another group at RPI is currently working on *in situ* experiments in ultrahigh vacuum chambers to address these issues.

CORA LIND

### High-Valence Cations Improve Hydration Resistance of MgO-CaO Materials

Improving the hydration resistance of magnesite and dolomite materials has important implications for the ceramics industry, particularly in the refractories sector where MgO-CaO bricks are often used to line basic open hearth furnaces. Research reported in the July issue of the *Journal of the American Ceramic Society* reveals that the addition of tri- and tetravalent cations in small proportions can improve hydration resistance by producing vacancies in solid solutions of CaO and MgO, and by substituting cations that are less prone to hydration.

Researchers at the East China University of Science and Technology in Shanghai and the Anshan Institute of Iron and Steel Technology pressed and fired high-density briquettes of flotation magnesite and dolomite doped with 0.5% (cation basis) of various monovalent to tetravalent cations. Dopants included NaF, NaCl, CaF<sub>2</sub>, MgCl<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, Cr<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, and ZrO<sub>2</sub>. Briquettes fabricated from analytically pure MgO and CaO were included