to using resources for research; they could always do more. As I pointed out in a previous letter, we must address this issue by setting priorities.

The final topic is the technical labor force—more specifically, the participation of women and underrepresented minorities. MRS has made great strides with regard to the participation of women and minorities in leadership roles; we are certainly ahead of the curve. I nevertheless want to discuss the issue with regard to underrepresented minorities in science and engineering. The margin of error in our experiments is larger than the fraction of underrepresented minorities getting degrees in science and engineering in the United States. In fact, some institutions have the same percentage (or less) of faculty of color now than they did 10 years ago. There is obviously work to be done. This is a responsibility that we all share; this is not a job for minority faculty—they alone are not effective. The Society needs to develop additional mechanisms that help to increase the participation and training (even at the elementary school level) of the diverse groups within its ranks.

Coordinating with other societies may prove to be an effective strategy. MRS members can have a strong influence on this issue, and we welcome input. Even simple things like keeping an open mind, or asking your local middle and high schools about the fraction of minority students placed in the appropriate classes that prepare them for college-level science classes; you might be surprised at the answer. The Society needs to take a long-term view, as it will involve a long-term investment.

As we look to the future, MRS needs to exploit all the exciting developments in the field of materials. Membership growth must occur in order for our Society to become an effective voice in the public and educational arena and, more importantly, for its longevity. I end by thanking each of you for the honor of serving as the 2006 MRS president.

PETER F. GREEN
2006 MRS President

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Research/Researchers

Semiconductor Nanocomposite
Designed to Enhance Exciton Emission of ZnO Nanorods

The high intensity of the defect emission band of ZnO nanostructures, related to O vacancies, has hampered their application in optoelectronic devices. J.M. Lin, C.L. Cheng, H.Y. Lin, and Y.F. Chen from the National Taiwan University enhanced the band edge emission of ZnO nanorods and substantially suppressed their defect emission by depositing SnO nanoparticles on their surface, as reported in the November 1 issue of Optics Letters (p. 3173). The SnO nanoparticles not only passivate the surface of ZnO nanorods, but also generate a transfer of carriers favored by the band alignment between the nanostructures of the semiconductors.

Using a tin metal target in a magnetron sputtering system, the researchers deposited SnO nanoparticles on hexagonal-shaped ZnO nanorods, 90–160 nm in diameter and 2 μm long, grown on a-orientated sapphire substrates through the vapor-liquid-solid mechanism in a vacuum tube furnace. They controlled the coverage of the SnO nanoparticles by varying the sputtering times.

Before deposition, the ZnO nanorods exhibited a weak UV exciton photoluminescence emission at 380 nm wavelength as well as more intense emission at 518 nm wavelength that is attributed to radiative relaxation through O vacancies. The UV exciton emission was enhanced 1200 times after deposition of the SnO nanoparticles, while the defect emission was quenched substantially. In addition to the surface modification of the ZnO nanorods generated by the strong chemical bonding between the SnO nanoparticles and the nanorod surface defects, which passivated the deep levels and avoided trapping of electrons, charge carrier transfer occurred from the SnO nanoparticles into the ZnO nanorods. Further evidence for this explanation was manifested by the reduction of the enhancement factor of the ZnO bandgap emission to only 200 times when the photon energy of the excitation was away from and below the bandgap of SnO nanoparticles. SnO nanoparticles deposited on quartz substrates also exhibit defect emission, which disappeared when the nanocomposite was formed, suggesting that the rate of transfer of carriers to ZnO nanorods was much faster than the rate of carriers being trapped in defects of SnO nanoparticles. Furthermore, not only can charge carriers in SnO nanoparticles transfer to ZnO nanorods, but also electrons in the defect level of ZnO nanorods can flow into the defect level of SnO nanoparticles, providing an additional channel for quenching the respective defect emissions.

The researchers said that this deposition process should be a useful approach for designing new nanocomposites for high-efficiency optoelectronic devices including fluorescent biolabels, light-emitting devices, and laser diodes.

JoAN J. CARVAJAL

Rubrene-Based Organic Single-Crystal FET Surpasses Performance of Conventional Organic Thin-Film Device

The possibility of integrating organic materials on flexible substrates may significantly influence consumer electronics. Despite the promise of organic electronics, inorganic materials remain the basis for wide-ranging applications like sensors and thin-film transistors. Progress in organic transistors has been slowed by the difficulty of synthesizing defect-free organic crystals. To overcome this obstacle, A.L. Briseno of the University of California, Los Angeles, Z. Bao of Stanford University, and their colleagues have fabricated organic single crystals as thin as 150 nm and as large as 1 cm × 1 cm. The single-crystal field-effect transistors (FETs) yielded mobilities as high as 4.6 cm²/V·s and on/off ratios of ~10⁴. The results were reported in the September issue of Advanced Materials (p. 2320; DOI: 10.1002/adma.200600634).

The researchers used physical vapor transport to grow the rubrene single crystals in the presence of argon from commercially available precursors. Two types of single-crystal devices were tested: a conventional, rigid device on a heavily doped silicon substrate with a 300 nm SiO₂ layer and flexible devices on either a polyimide Kapton film or poly(ethylene terephthalate) (PET) substrate. In both cases, bottom-contact source-drain electrodes were used. The rigid substrates used gold modified with 4-nitrobenzenethiol (NB) for enhanced charge injection for source and drain electrodes. For the flexible devices, either gold or indium tin oxide (ITO) was used as the gate electrode, and gold was used for source and drain electrodes. The gate and the source and drain regions were separated by silicon dioxide in the con-
A plot of mobility versus gate voltage showed no dependence on gate voltage beyond -20 V. The researchers believe that gate-voltage dependence is related to the presence of interfacial defects or grain boundaries in polycrystalline thin films. Atomic force microscopy scans revealed that smooth (surface roughness, $<0.23$ nm), virtually step-free crystals can be obtained for crystal thicknesses of less than 1 μm. As the thickness of the organic crystal increased, the mobility steadily decreased. The researchers said the decrease in mobility is due to poor conformability of thicker crystals. The researchers further said that the proof of the robustness of the device is their finding that the mobility is restored to 91.3% of the original value after releasing the flexible substrate from a bending radius of 5.9 mm. No damage was noticeable on the rubrene single crystals even after this severe bending.

Jeremiah T. Abiade

Cultural and Biological Evolutionary Concepts Combined to Solve Crystal Structures from Powder Diffraction Data

Biological evolutionary concepts have in recent decades been used to develop computational techniques for global optimization problems in chemistry, nanotechnology, and bioinformatics. Differential evolution (DE), for example, has been effective in several areas of crystal structure determination. Cultural evolution in a society, however, is much faster than biological evolution. Recently, S.Y. Chong and M. Tremayne at the School of Chemistry, University of Birmingham, U.K., incorporated principles based on human social evolution into a DE global optimization method, thereby substantially increasing computational efficiency. The researchers' new method, which they call cultural differential evolution (CDE), is the first application of cultural evolution concepts in a chemical or crystallographic context.

As reported in a recent issue of Chemical Communications (p. 4078; DOI: 10.1039/b609138e), Chong and Tremayne compared DE and CDE global optimization algorithms used to solve two crystal structures from powder diffraction data. The model consisted of the molecule (excluding hydrogens whose intramolecular conformation cannot be uniquely defined) in a unit cell. In each algorithm, the initial population of trial structures was generated randomly. Child structures were created by recombining and mutating parent structures. The population was updated by comparing children to parents and applying fitness criteria. The variables to be optimized were the molecule's position, orientation, and internal torsional angles (standard bond lengths and valence angles are used, although they could also be included as variables). In DE, each variable was reset to a point between the parent's value and a static boundary value if the child value exceeded the boundary. However, as generations are spawned, these variables display population clustering—generational information that is used in the CDE algorithm to guide the optimization by implementation of dynamic boundaries, which restrict the search and effectively prune population space.

Chong and Tremayne showed that their CDE algorithm converged up to 54% more quickly than DE for a test case—the molecule baicalein. The second case was an unknown crystal structure—methyl-propyl succinimide. CDE obtained the structure corresponding to the global minimum in 461 generations, while DE required 988. The researchers said that the crystal structure contained stacks of centrosymmetric dimers linked into layers (see Figure 1).

Chong and Tremayne said it is “remarkable that implementation of such a simple concept as cultural evolution has such a dramatic effect on the efficiency of our calculations. Work is now ongoing to optimize the relative proportion of the different ‘types’ of evolution within our calculation, and we plan to extend our method to other applications such as protein folding and diffuse scattering.”

Steven Trohalaki

Model of Magnetic Impurity Formation in Quantum Point Contacts May Explain the “0.7 Anomaly”

Nanoelectronics refers to electronic transport through miniaturized devices. The simplest such device, and the basic building block for more complicated devices, is a “quantum point contact,” a constriction connecting large electron reservoirs. Yigal Meir, a theoretical physicist at Ben-Gurion University of the Negev in Israel, has now developed an explanation of the “0.7 anomaly,” a feature in the conductance of quantum point contacts that has eluded explanation for almost 20 years. Meir’s findings are published in the August 24 issue of Nature (p. 900, DOI:10.1038/nature05054).

According to quantum mechanics, and the wavelike nature of electrons, scientists expected the conductance through such a device to increase as the gap grew bigger by integer steps of universal value. While this was found to be true in early experiments, surprisingly, an additional first step, approximately 0.7 times the expected...
universal value, had also been observed, which scientists first attributed to irregularities in the device (“the 0.7 anomaly,” as it became known).

While visiting Princeton University, Meir and his host, Ned Wingreen, theorized the existence of a magnetic impurity, a localized electron, in a quantum point contact to explain the 0.7 anomaly. While their theoretical calculations explained its temperature and magnetic-field dependence, identification of the proposed impurity was still needed to overcome skepticism in the physics community about how a magnetic moment could form in such a system.

“The classical analogy of a quantum point contact is a sea of electrons around a hill,” Meir said. “The existence of a magnetic impurity on the point of contact is equivalent to the formation of a puddle of water at the top of the hill—a counterintuitive phenomenon.”

In the Nature article, published with his Ben-Gurion University postdoc, Tomaz Rejec, Meir attributes the emergence of the magnetic impurity to the attraction of electrons toward the lower electron density at the vicinity of the quantum point contact, a process known as screening. Extensive numerical calculations show that the wavy nature of these electrons then causes the 0.7 anomaly.

“This is both good and bad news for quantum computer devices based on quantum dots which require that no outside factors affect the circuits,” Meir said. “Magnetic impurities at point contacts would render such computer devices inoperable. However, the magnetic impurity is formed only when conductance through the point of contact is around 0.7, so setting the conductance of each contact below that value should allow a circuit formed by quantum dots to function.”

Thin-Film Coatings of Oppositely Charged Nanoparticles Fabricated Using Layer-by-Layer Deposition

Electrodeposition of semiconductors and metal nanoparticles and sol-gel chemistry-based deposition of nanoparticles are among the methods currently used for thin-film coating onto various substrates. However, attempts to produce conformal thin-film coatings containing two or more nanoparticles onto various geometric surfaces has been unsuccessful. In 1966, R.K. Iler introduced the layer-by-layer (LBL) deposition method that was used to create multilayers of inorganic “colloidal particles.” He concluded that thin films of oppositely charged nanoparticles could be formed onto substrates from aqueous suspensions. In 1991, G. Decher and colleagues began to use LBL processing to produce multilayer thin films of oppositely charged polyelectrolytes. Now, R.E. Cohen, M.F. Rubner, and D. Lee from the Massachusetts Institute of Technology have reexamined the LBL method to fabricate thin-film coatings of oppositely charged nanoparticles in films without polyelectrolytes.

As the research team reported in the October issue of Nano Letters (p. 2305; DOI: 10.1021/nl061776m), multilayer coatings consisting of bilayers with one layer containing nanoparticles of TiO₂ and the next layer containing nanoparticles of SiO₂ were fabricated onto glass or silicon substrates. Sequential adsorption of the nanoparticles was performed by first cleaning the substrate, dip-coating it in a nanoparticle aqueous suspension at pH 3, and rinsing the coated substrate in deionized water for 4 min.

To characterize the thin-film coatings, the researchers used a spectroscopic ellipsometer to determine the film thickness. The researchers used a modified ellipsometry method to measure the porosity and composition of the coating and validated this technique using a quartz crystal microbalance and X-ray photoelectron spectroscopy.

A linear growth behavior was observed when multilayers of the nanoparticles were coated onto the different substrates. The researchers said that the linear behavior of the multilayer might result from the complete coating and uniformity of the surface.

Lee and co-workers also found a major difference between the porosity of the 7-nm TiO₂/22-nm SiO₂ and the 7-nm TiO₂/7-nm SiO₂ nanoparticle-based multilayer films. Denser packing of the nanoparticles in films was observed in the latter sample compared with the former (with 22-nm SiO₂ nanoparticles).

The researchers said that the thin-film coatings of TiO₂ and SiO₂ nanoparticles exhibited potential in applications where antireflection, antifoaming, or self-cleaning properties are preferred.

Olaomo Moloye

Model Predicts that Quantum-Correlated Photon Pairs Produced in Silica Waveguides Evade Limits of Spontaneous Raman Scattering

Quantum-correlated photon pairs are useful for a variety of quantum information applications, including quantum cryptography and quantum computation. To date, the standard technique for generating these pairs has been parametric down-conversion (PDC) of short-wavelength light in nonlinear optical crystals. Recently, a number of groups have shown that four-wave-mixing (4WM) in silica optical fibers can generate high-quality quantum-correlated photon pairs with much higher spectral brightness than achievable by PDC, but this approach appears to be limited by spontaneous Raman scattering (SRS) in the amorphous silica. In the November 1 issue of Optics Letters (p. 3140), Q. Lin and G.P. Agrawal of the University of Rochester proposed a new scheme for generating correlated photon pairs in waveguides of crystalline silicon that should retain the advantages of silica fibers while eliminating the effects of SRS.

Although classical optics predicts that the intensities of two laser beams emerging from a 50/50 beamsplitter are correlated, this is not true for single photons. The indivisibility of the photon means that each photon arriving at a 50/50 beamsplitter chooses one of the two output paths, leading to a loss of correlations at the quantum level. The techniques of PDC and 4WM generate quantum-correlated photon pairs by producing them two at a time through nonlinear interactions. In the case of amorphous silica, the ultimate limitation on this pairwise production is the unpaired photons from SRS.

The researchers proposed using a silicon waveguide conventionally fabricated along the [110] direction on the (001) surface. They then modeled the 4WM generation of photon pairs by a single cw pump at 1550 nm, including the effects of free carrier absorption and two-photon absorption. For a pump polarized in the transverse magnetic (TM) mode, SRS is prohibited by the symmetry of crystalline silicon, and the model calculations indicate that for relatively low pump intensities, free carrier absorption and two-photon absorption also play minor roles. For typical parameters, the quantum correlations can exceed 30 (that is, the number of paired photons is 30 times larger than that of unpaired photons), while the spectral brightness remains as high as 2 × 10⁸ pairs/s/GHz/mW. These values are comparable to the best available from conventional silica fibers but have no SRS component. They are also competitive with systems based on PDC in periodically poled LiNbO₃ waveguides, but the proposed silicon waveguide system would not have the same complicated fabrication and stringent temperature control requirements. Given these theoretical results and the ease of fabrication of such a system, 4WM in silicon waveguides may soon become a standard technique for producing high-quality quantum-correlated photon pairs.

Colin McCormick
Quantum Coherence Possible in Incommensurate Electronic Systems

A team of researchers led by T.-C. Chiang at the University of Illinois at Urbana-Champaign has demonstrated that quantum coherence is possible in electronic systems that are incommensurate, thereby removing one obstacle in the development of quantum devices.

Electronic effects in thin films and at interfaces lie at the heart of modern solid-state electronic technology, according to the researchers. As device dimensions shrink toward the nanoscale, quantum coherence and interference phenomena become increasingly important.

“At quantum dimensions, quantum mechanics says device components will couple together and act in a concerted manner, where everything affects everything else,” said Chiang, a professor of physics and a researcher at the university’s Frederick Seitz Materials Research Laboratory. “Most scientists assume that electronic layers must be commensurate, so electrons will flow without being diverted or scattered.”

In fact, however, most material interfaces are incommensurate as a result of differences in crystal size, symmetry, or atomic spacing, Chiang said. Random scattering of electrons was thought to destroy quantum coherence in such systems at the nanoscale.

Now, by studying electron fringe structure in silver films on highly doped silicon substrates, Chiang and his research group—N. Speer, S.-J. Tang, and T. Miller—have showed that even when electronic layers are incommensurate, they can still be coherent. The researchers reported their findings in the November 3 issue of Science (p. 804, DOI: 10.1126/science.1132941).

The researchers grew atomically uniform silver films that were a few monolayers thick on highly doped n-type silicon substrates. Then they used angle-resolved photoemission to examine the fine-structure of the electronic fringes. This technique probes the first 2–3 atomic layers, but is sensitive to the substrate because the wavefunction sampled by the photoemission process encompasses the silver film and a few tens of atomic layers of the silicon.

Although the silver films and silicon substrates are lattice-mismatched and incommensurate, the wave functions are compatible and can be matched over the interface plane, Chiang said. The resulting state is coherent throughout the entire system.

The fringes the scientists recorded correspond to electronic states extending over the silver film as a quantum well and reaching into the silicon substrate as a quantum slope, with the two parts coherently coupled through an incommensurate interface structure.

“An important conclusion drawn from the present study is that coherent wave function engineering, as is traditionally carried out in lattice-matched epitaxial systems, is possible for incommensurate systems,” the researchers wrote, “which can substantially broaden the selection of materials useful for coherent device architecture.”

Nanoporous Au Approaches Yield Strength of Bulk Material

Gold has long been a coveted material for use in jewelry and commerce because of its lustrous appearance and scarcity in nature. Recent reports have generated considerable interest in nanostructured Au for use in sensors, actuators, and catalysis. However, the mechanical properties of nanostructured—particularly, nanoporous —metal foams are not well understood. In the October issue of Nano Letters (p. 2379; DOI: 10.1021/nl601978i), J. Biener of Lawrence Livermore National Laboratory in California, C.A. Volkert of Institute for Materials Research II in Karlsruhe, Germany, and their colleagues reported that the yield strength of nanoporous gold (np-Au) may exceed bulk values. The researchers suggested that the nanoporous metal foams can be envisioned as a three-dimensional network of ultrahigh-strength nanowires (i.e., ligaments).

Disk-shaped samples of np-Au with relative densities of 0.25 and 0.3 (diameter, ~5 mm; thickness, ~300 μm) were prepared by selective dissolution of silver from Ag0.75Au0.25 and Ag0.5Au0.5 alloys, respectively. Nanoporous Au foams with 25-nm and 50-nm ligaments were prepared by immersion in concentrated nitric acid. The pore size was adjusted by varying the dealloying conditions. Nanoporous Au with 10-nm ligaments was prepared by electrochemical dealloying. Energy-dispersive x-ray spectroscopy was used for compositional analysis, and scanning electron microscopy was used to determine pore/ligament size. The researchers used a combination of nanoindentation, column microcompression, and molecular dynamics simulation to investigate the size-dependent properties of nanoporous gold.

According to nanoindentation studies, np-Au with a relative density of 25% shows an increase in strength with decreasing ligament diameter. The researchers reported an increase in yield strength from ~33 MPa to ~171 MPa as the ligament diameter was decreased from 50 nm to 10 nm, which is comparable to the value for bulk Au (~30–200 MPa). The 10-nm ligament sample had a porosity of ~75%, bringing together two conflicting properties, high strength and high porosity. This result was confirmed by microcompression tests on micron-sized nanoporous Au columns with an aspect ratio of 2. Molecular dynamics simulations confirmed the high yield strength of nanometer-sized Au ligaments but failed to reproduce the experimentally observed size effect. The researchers said that the experimentally observed increase in strength with decreasing size can be linked to the presence of defects.

Jeremiah T. Abade

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