ventional device and poly-4-vinylphenol (PVP) in the flexible device. The single crystals were then electrostatically bonded onto the contacts.

The performance of single crystals on the rigid and flexible substrates was tested. 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

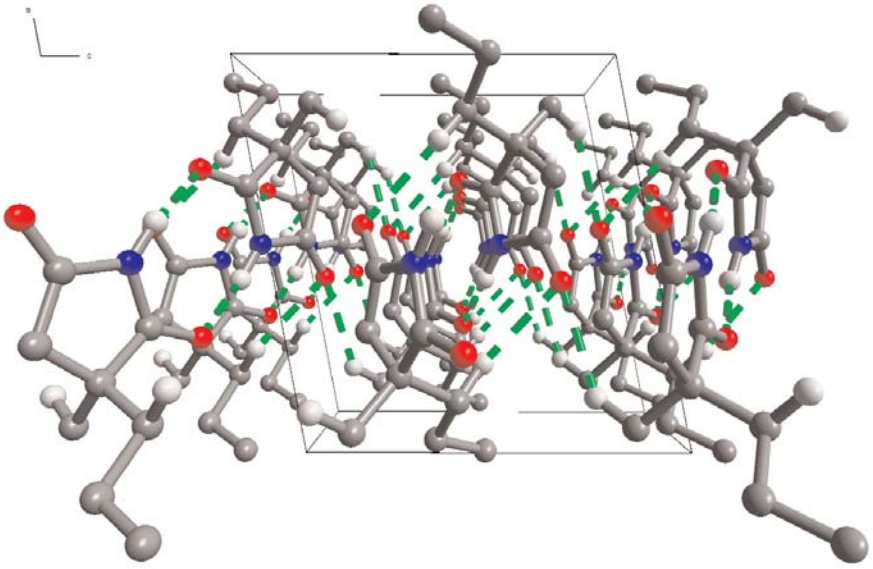

Figure 1. The crystal structure of α-methyl-α-propyl succinimide contains stacks of centrosymmetric dimers linked into layers. Hydrogen bonding is indicated by green dashed lines. Oxygen atoms are red; carbon, grey; hydrogen, light grey; and nitrogen, blue. Reproduced with permission from Chem. Commun. (39) (2006) p. 4078; DOI: 10.1039/b609138e; © 2006 Royal Society of Chemistry.

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—α-methyl-α-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 counter-intuitive 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 TiO_2 and the next layer containing nanoparticles of SiO_2 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 TiO_2/22-nm SiO_2 and the 7-nm TiO_2/7-nm SiO_2 nanoparticle-based multilayer films. Denser packing of the nanoparticles in films was observed in the latter sample compared with the former (with 22-nm SiO_2 nanoparticles).

The researchers said that the thin-film coatings of TiO_2 and SiO_2 nanoparticles exhibited potential in applications where antireflection, antifogging, or self-cleaning properties are preferred.

OLAJOMPO MOLOYE

Model Predicts that Quantum-Correlated Photon Pairs Produced in Si 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 $[\bar{1}10]$ 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 2×10^5 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 $LiNbO_3$ 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