Ab Initio Study of Polonium Reveals Origins of Simple Cubic Structure

Polonium is a rare radioactive element that has potential for a variety of engineering applications from thermoelectric power generation to dust removal and elimination of static charges. Recently, polonium has been covered in news outlets after being found in cigarettes as well as some herbal teas, and because of its nefarious use in the poisoning of Alexander Litvinenko. Beyond its notoriety, polonium is unique among all elements as being the only elemental solid found with a simple cubic crystal structure. Researchers at the Institute of Physics of Materials and Masaryk University in the Czech Republic report on *ab initio* calculations that explain this unique structure as a result of the Darwin and mass-velocity relativistic interactions, but not spin-orbital coupling. As an intense alpha emitter, experimental exploration of polonium is difficult, but these simulations, appearing in the July 6 issue of *Physical Review Letters* (016402/1-4, DOI: 10.1103/PhysRevLett.99.016402) describe new phases in pressure regimes that should encourage work with this difficult material.

D. Legut, M. Friák, and M. Šob employ a local density approximation potential combined with relativistic effects to simulate polonium in equilibrium and stressed states. Energy profile calculations, seen in Figure 1, at increased pressures demonstrate a collapse of the energy minimum associated with simple cubic structure. These calculations express the energy as a function of the trigonal deformation path.

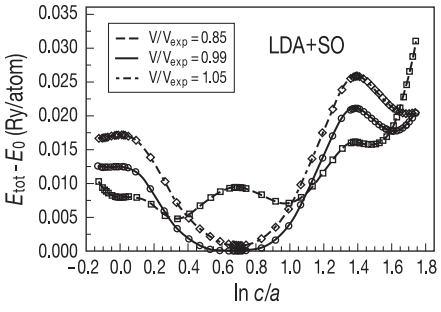

Figure 1. Local density approximation energy profiles for polonium at various stress levels. Ln c/a = 0.693 corresponds to a simple cubic structure, for a trigonal deformation path with c in the [111] direction and a along a perpendicular axis. At higher pressures, the simple cubic structure destabilizes, and minima are observed corresponding to trigonal formations. Reprinted with permission from D. Legut, M. Friák, and M. Šob, *Phys. Rev. Lett.* **99**, 016402 (2007).

A bimodal state comprised of trigonal structures, similar to the high temperature β phase of polonium as well as the structures of isoelectronic tellurium and selenium, is predicted at pressures of 1–3 GPa.

The researchers then investigated the equilibrium simple cubic structure by comparing electronic structure calculations between polonium and tellurium while varying the relativistic factors active in the calculation. The spin-orbital coupling was found to not be of critical importance to achieving simple cubic structure, but the other relativistic effects were. The researchers said that the contributions from the mass-velocity term and the Darwin term, a quantum perturbation, grow larger more quickly than the spin-orbit term for larger elements in the same periodic group. These results provide a comprehensive explanation of the special combination of relativistic factors that combine to give polonium a simple cubic structure. Additionally, by predicting a bimodal phase within a narrow pressure regime, the researchers give focus to difficult experiments that may provide fruitful results.

ARTHUR FELDMAN

Enzymes Can Cut or Glue Nanoparticle-Coated DNA

Applying techniques inspired by Mother Nature, scientists can precisely construct materials at the nanometer scale. To this end, many studies have focused on using biomolecules (e.g., DNA) as templates to produce materials with specific sizes and shapes. DNA is a chain-like biopolymer with intrinsic biological functions such as self-identification, site-specific cleavage or ligation by restriction enzymes. However, one challenge is whether DNA hybridized with nanomaterials can still be manipulated by enzymes. A group of researchers at Purdue University have found that site-specific cleavage and ligation of DNA coated with nanoparticles can still occur.

As described in the July 24 issue of *Chemistry of Materials* (p. 3586; DOI: 10.1021/cm070850e), A. Ivanisevic and co-workers demonstrated cleaving and ligation of nanoparticle-coated DNA using enzymes. The researchers were able to prepare $CoFe_2O_4$ nanoparticles coated with λ phage DNA by incubating λ phage DNA in a Tris buffer solution of 3.5 nm 2-pyrrolidinone-capped $CoFe_2O_4$ nanoparticles. Following the synthesis, they cleaved the hybrid with BamH1 and EcoR1 and then ligated the fragments with T4 ligase.

The researchers evaluated the effect of the digestion and ligation by gel electrophoresis and UV-vis spectroscopy. Digested samples with various concentrations of nanoparticles were run on an agarose gel. The samples coated with nanoparticles produced all of the fragments expected from cleavage of the DNA sample only. This result demonstrated that the enzymes could still cut the DNA, even though it was coated with nanoparticles. The researchers also observed that the fluorescent intensity of the samples decreased with increasing nanoparticle concentration. Further experiments by UV-vis spectroscopy suggested that this effect was caused by the conformation change of the DNA. In the next step, the researchers successfully ligated the DNA fragments. Similarly to the digestion samples, the ligation samples experienced a conformation change due to the increased concentration of nanoparticles. The researchers concluded that the nanoparticle coating will not affect enzyme activity on the DNA. The researchers believe that this finding will open up methods to generate novel one-dimensional nanomaterials, which may have applications "in memory storage devices and magnetic field sensors and can provide platforms for fundamental studies of magnetic tunneling junction devices."

CHANG ZHONG

Compact Polarization Rotator May Help Enable Integrated Microphotonic Systems

The emerging class of microphotonic devices, which carry information with photons rather than electrons, may enable entire categories of novel applications from optical computers to chip-scale integrated photonic circuits. But photons have one crucial difference from electrons in standard semiconductor circuits: they are polarized, and as microphotonic devices shrink it becomes increasingly important to control this polarization at miniaturized scales. In an aticle in the August issue of *Optics Letters* (p. 2176), D. Beggs and T. Krauss of the University of St. Andrews, Scotland, and M. Midrio of the Universita degli Studi di Udine, Italy, report the fabrication of a new compact polarization-rotation device that should enable better polarization control in microphotonic systems.

Photon polarization is a problem in microphotonic devices because the response of small-sized waveguides built from standard silicon or III–V semiconductors to different polarizations can vary widely. To help control this, a number of passive polarization-rotation devices have been demonstrated, based either on mode evolution or birefringence. Unfortunately, devices based on mode evolution tend to

be too long for practical use, and those based on birefringence, while small, are too lossy to be practical. To address this, the researchers decided to pursue a hybrid device, which combines a central birefringent section with mode-matching tapered-waveguide input/output couplers to reduce optical loss. The researchers fabricated samples of the devices in an InGaAsP heterostructure consisting of an InP top cladding layer, an InGaAsP waveguide layer, and an InP buffer layer. A silica layer was deposited to form a hard mask. The waveguide was formed by writing the waveguide pattern into a 200-nm thick layer of polymethylmethacylate (PMMA) using electron-beam lithography, transferring the pattern into a hard-mask layer of silica with reactive ion etching using CHF_3 chemistry, and finally deep etching into the InP layers using chemically assisted ion beam etching. The final devices were all less than 50 μm long.

The group then tested the devices by launching polarized light at a wavelength of 1.55 μm into them and measuring the rotation of the plane of polarization as a function of the width of the central birefringent section. The rotation angle increased with decreasing width, and ranged from nearly zero for a 1500-nm-wide central section to over 250 degrees for a 500-nm-wide central section. The overall insertion losses were only about 1 dB, dominated by propagation loss rather than back reflections, which can degrade photonic circuit performance. The devices were also found to operate over a 100 nm wavelength range, demonstrating that they could be used in a broadband photonic circuit configuration. Given these results, hybrid polarization-control devices of this nature may form a key component of future integrated microphotonic systems.

COLIN MCCORMICK

SnO_2 Nanowires Used to Fabricate Fully Transparent Thin-Film Transistor Devices

The extraordinary properties of semiconductor nanowires have led many researchers to pursue novel device applications. For example, conventional transparent thin-film transistors (TFTs) that use single-crystal channel materials typically require growth and annealing at high temperature and expensive single-crystalline substrates. In contrast, high-performance, nanowire-based TFTs have been fabricated on glass and plastic substrates. A key advantage to this approach is its capacity to separate the nanowire growth step from the device fabrication, which makes moot the compatibility between the device substrate with nanowire growth. High temperatures can therefore be used to obtain nanowires composed of single crystals, which are then transferred to the device substrate, configured into thin-film form, and processed into TFTs using conventional techniques. Heretofore, opaque semiconducting nanowires, (e.g., silicon), were used with electrodes made from normal metals such as Au or Ni but new frontiers such as "invisible electronics" require optical transparency. Recently, W. Lu and co-researchers from the University of Michigan fabricated fully transparent nanowire-based TFT devices that exhibit excellent transistor performance.

As reported in the August issue of *Nano Letters* (p. 2463, DOI: 10.1021/nl0712217), Lu and co-researchers grew single-crystalline, Ta-doped SnO_2 nanowires using a simple, inexpensive method and used them as channel material in field-effect transistor (FET) and TFT devices. The researchers chose SnO_2 nanowires because they have high optical transmittance and easily form Ohmic contacts with conducting oxide films. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) showed that the nanowires have a mean, uniform diameter of 55 nm with lengths measured in the tens of micrometers. High-resolution TEM showed that each nanowire is a perfect single crystal. FET devices with a channel consisting of a single nanowire, fabricated on Si substrates to investigate the intrinsic electrical properties of Ta-doped SnO_2 nanowires, displayed field-effect mobilities over 100 $cm^2/V\text{-}s$. In contrast, undoped SnO_2-nanowire devices displayed pronounced Schottky barrier behavior. The researchers then fabricated fully transparent TFTs on glass substrates using arrays of parallel, doped nanowires as the transistor channel and indium tin oxide source and drain electrodes. Techniques, such as sputter deposition, that can be used in large-scale production were employed. Furthermore, the high-temperature limit in the fabrication process was 250°C, making it compatible with many plastic substrates. Even at low nanowire coverage, the TFTs exhibit high mobilities similar to the single-nanowire devices as well as excellent optical transparency and transistor performance, such as transconductance, bias, voltage range, and on/off ratio. The researchers said that "[our] study circumvents the position-registry problem hindering single-nanowire based approaches and may lead to large-scale applications of high performance, transparent, nanowire-based thin-film devices on diverse substrates."

STEVEN TROHALAKI

Carbon Nanotubes Endure Heavy Wear and Tear

The ability of carbon nanotubes to withstand repeated stress yet retain their structural and mechanical integrity is similar to the behavior of soft tissue, according to researchers J. Suhr of the University of Nevada in Reno, V. Pushparaj of Rensselaer Polytechnic Institute, and their colleagues.

When paired with the strong electrical conductivity of carbon nanotubes, this ability to endure wear and tear, or fatigue, suggests the materials could be used to create structures that mimic artificial muscles or electromechanical systems, the researchers said.

"The idea was to show how fatigue affects nanotube structures over the lifetime of a device that incorporates carbon nanotubes," said Pushparaj, a senior research specialist in Rensselaer's department of materials science and engineering. "Even when exposed to high levels of stress, the nanotubes held up extremely well. The behavior is reminiscent of the mechanics of soft tissues, such as a shoulder muscle or stomach wall, which expand and contract millions of times over a human lifetime."

As reported in the July issue of *Nature Nanotechnology* (p. 417; DOI: 10.1038/nnano.2007.186), the research team created a free-standing, macroscopic, 2-mm square block of carbon nanotubes, made up of individual, vertically aligned, multi-walled nanotubes. The researchers then compressed the block between two steel plates in a vice-like machine.

The team repeated this process more than 500,000 times, recording precisely how much force was required to compress the nanotube block down to about 25% percent of its original height. Even after 500,000 compressions, the nanotube block retained its original shape and mechanical properties, the researchers said. Similarly, the nanotube block also retained its original electrical conductance.

In the initial stages of the experiment, the force needed to compress the nanotube block decreased slightly, but soon stabilized to a constant value, said Suhr, an assistant professor of mechanical engineering at the University of Nevada.

As the researchers continued to compress the block, the individual nanotube arrays collectively and gradually adjusted to getting squeezed, showing very little fatigue. This "shape memory," or viscoelastic-like behavior—although the individual nanotubes are not themselves viscoelastic—is often observed in soft-tissue materials.

While more promising than polymers and other engineered materials that exhib-