more regularly spaced, whereas the ones obtained from nanoparticles without ligands have a larger mean diameter and a broad dispersion of diameters. The UV-ozone treatment itself leaves the Ni nanoparticle core sizes unchanged, but during heating to 700°C, particles without ligands agglomerate and coalesce, which results in polydisperse seeds for nanofiber growth. Coalescence occurs only prior to nanofiber growth: Once growth is initiated, no further coalescence can occur, and the fibers grow separately.

The researchers have also demonstrated the formation of graphitic shells around the ligand-capped particles during the pre-growth heating. The shells are made of the carbon atoms from the ligand molecules. They protect the particles from agglomeration and also serve as a carbon source for the initial stage of carbon nanofiber growth.

Elsa Couderc

Nano Focus

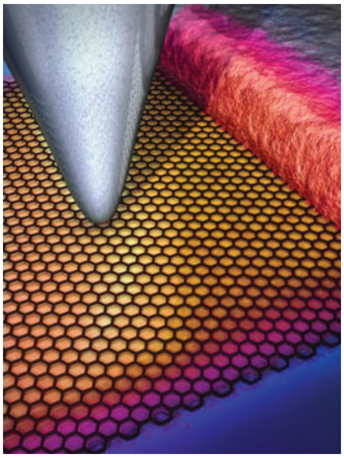
Self-cooling observed in graphene electronics

Cooling electronic devices such as computers consumes a great deal of energy, typically in the form of air or water cooling. But what if the materials used in making the electronics cooled themselves during operation? Recent findings by William King and Eric Pop of the University of Illinois, Urbana-Champaign, published April 3rd in the online journal *Nature Nanotechnology* (DOI: 10.1038/nnano.2011.39), suggest that graphene components may be able to do just that.

Using a method they developed to measure the nanoscale temperature distribution with atomic force microscopy (AFM) tips, they were able to determine the temperature distribution in a working graphene field-effect transistor (FET) with a spatial resolution of about 10 nm and a thermal resolution of about 0.25°C. They used this data to construct temperature maps of the FET. "The first thing that was remarkable to me," King said, "was that we could actually measure the temperature of a working FET where the device layer was just 1 atom thick."

By feeding temperature data from these maps into a simulation program developed by Pop, they discovered that the temperature rise at a graphene/metal junction in the circuit differed depending on the direction of current flow through the device. In fact, they found a thermoelectric "nanoscale cooling" effect that accounted for about one-third of the temperature difference; the rest was due to resistive heating.

Additional simulations that looked at possible future improvements in graphene materials and metal contacts showed further promise for self-cooling electronics. "If graphene improves in the way that everyone thinks it will, the thermoelectric effect will grow in importance, and the resistive heating will shrink," King said. "Projecting forward to carbon electronics of the future, the thermoelectric cooling effect will govern everything about the contacts."



An atomic force microscope tip scans the surface of a graphene/metal contact to measure temperature with spatial resolution of about 10 nm and temperature resolution of about 250 mK. Color represents temperature data. *Credit*: Alex Jerez, Beckman Institute Imaging Technology Group

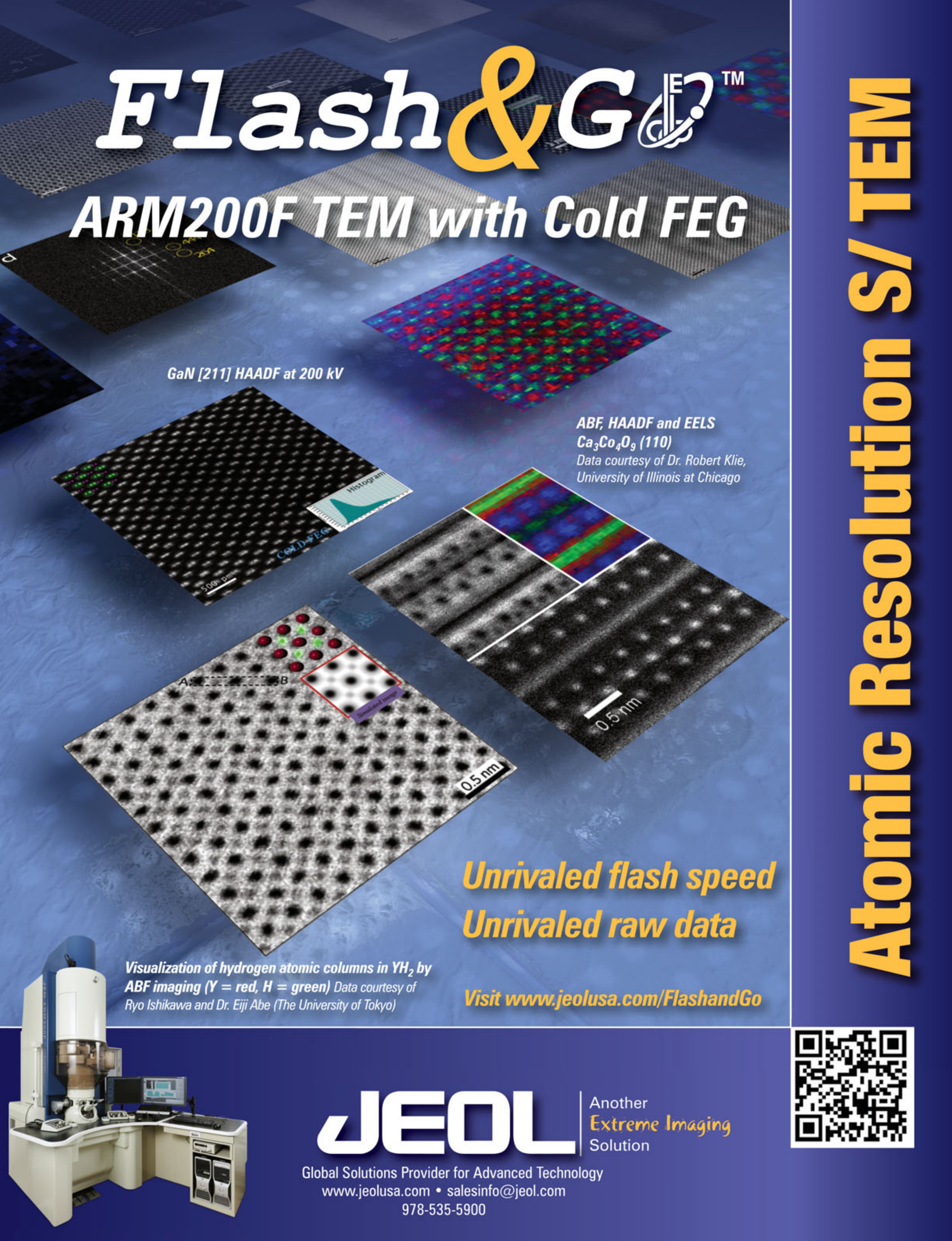
Tim Palucka

Computational method used to construct database of new zeolite-like materials

Industrial applications for zeolites include catalysis, ion exchange, and separations. The scope of applicability would increase with the discovery of new zeolites (currently fewer than 200 zeolites are known), which can be stimulated with computational predictions of stable, zeolite-like structures. Recently, R.S. Pophale and M.W. Deem of Rice University, in collaboration with P.A. Cheeseman of Purdue University, refined their previously published computational approach by accounting for the Pauli exclusion principle, and constructed a database of predicted, zeolite-like materials.

As reported recently in the online edition of *Physical Chemistry Chemical Physics* (DOI: 10.1039/c0cp02255a), Pophale, Cheeseman, and Deem developed a Monte Carlo technique to randomly sample the structural space of low-energy, zeolite-like structures. Geometry optimizations were performed with two interatomic potentials—the Sanders-Leslie-Catlow potential, which is accurate for zeolites, and the van Beest-Kramer-van Santen potential, which agrees well with experimentally determined enthalpies of formation. Enforcing the Pauli exclusion principle makes the structures resulting from the two potentials much more realistic, stable, and similar to each other.

Over 2.6 M zeolite-like structures were found and about 10% have energies in the range of known zeolites. Calculated powder x-ray diffraction patterns for the database structures are similar to those of known zeolites.


Histogram
COLD FEG
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A
B
Simulated image
0.5 nm

The researchers said that the low-density structures in their database are of particular interest because they expect them to have large rings and large pores, and expressed the hope that their work will spur attempts at their synthesis. The researchers also said that they are collaborating with other research groups in order to explore the adsorption and diffusion of small molecules in a subset of their zeolite database as well as how their predicted zeolites can be used for carbon sequestration.

The researchers said that their approach "may serve as a guide for construction of analogous databases for other materials such as metal-organic frameworks or crystal hydrates. Diversity in structures and possible functionality among these classes of materials could reveal themselves through such efforts."

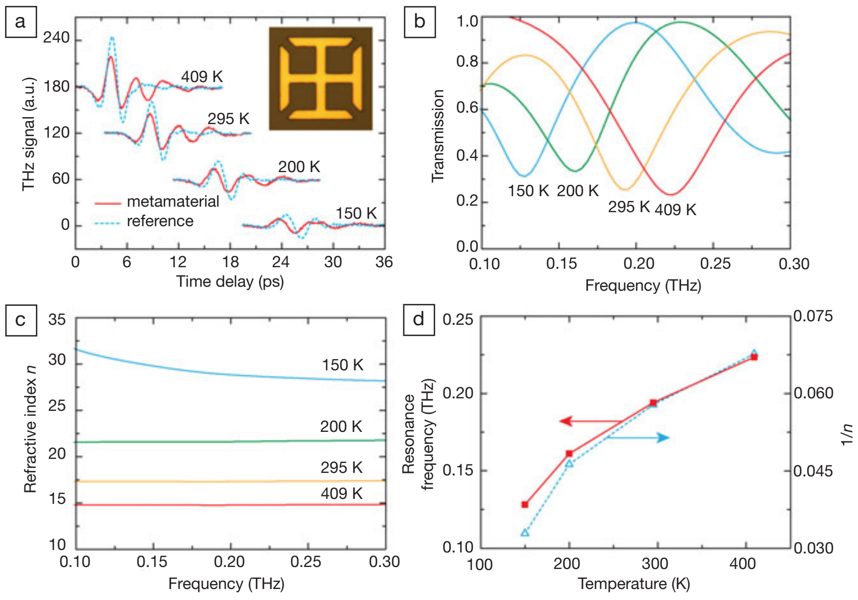
Steven Trohalaki

Nano Focus

Thermal tunability in terahertz metamaterial achieved on strontium titanate single crystals

Although split-ring resonator (SRR) based metamaterials are attractive for use in devices with novel functionalities over a large electromagnetic spectral domain, devices incorporating SRRs fall short on performance due to lack of dynamic control over their resonances. R. Singh, H.-T. Chen, and co-researchers at the Center for Integrated Nanotechnologies at the Los Alamos National Laboratory, hypothesized that in most cases the frequency tuning of metamaterial resonance is accompanied with a large variation in resonance strength, which is undesirable and caused by the damping from the materials integrated in metamaterials.

As reported in the April 7th issue of *Optics Letters* (DOI: 10.1364/OL.36.001230; p. 1230), the researchers fabricated a planar square array of subwavelength 200-nm-thick gold electric SRRs on a 533-μm-thick single crystal (100) oriented strontium titanate (STO) substrate. They measured the resonant behavior in the THz frequency range of the metamaterial as a function of temperature using a time-domain spectroscopy (TDS) system incorporated with a continuous flow liquid helium cryostat. The researchers observed a 43% shift in resonance frequency after cooling the metamaterial from 409 K to 150 K with less disparity in resonance strength. They attributed this behavior to the temperature-dependant dielectric constant of strontium titanate.



At various temperatures, (a) THz pulse in the time-domain after transmission through the metamaterial and a bare strontium titanate (STO) substrate, (b) normalized THz transmission amplitude spectra through the metamaterial, (c) refractive index of the STO substrate as a function of THz frequency, and (d) a comparison of resonance frequency and inverse of STO refractive index. Inset to (a) is the microscopy image of a metamaterial unit cell. Reproduced with permission from *Opt. Lett.* **36** (7) (2011) DOI: 10.1364/OL.36.001230; p. 1230. © 2011 Optical Society of America.

The experiment opens up avenues for designing tunable terahertz devices by exploiting the temperature-sensitive characteristics of high dielectric constant substrates and complex metal oxide materials. Such thermal tuning of metamaterial resonance using STO and ferroelectric materials will enable the integration of metamaterials with other complex metal oxides and resonance tuning approaches to realize multifunctional THz metamaterial devices.

Jean L. Njoroge