grew on each Ni tip, the field-emission measurements were specific to individual nanotubes for two reasons. First, the emission current (I_{FE}) is an exponential function of field, so only a few MWNTs are able to emit. Second, the geometry of field emission allows the contributions of each MWNT to the field-emission pattern to be easily distinguished.

The researchers determined the temperature and resistance from TEDs obtained for various I_{FE}. As I_{FE} increased, the TEDs became broader and shifted to lower energy. The broadening is partly explained by the rise in the temperature due to Joule heating along the MWNTs. The shift to lower energy results from an IR drop along the tube.

ELIZABETH SHACK

Carbon Nanotube Bandgaps Manipulated with Metallofullerenes

A team of researchers from Seoul National University, Soongsil University, and Nagoya University has detected localized bandgap-energy changes in single-walled carbon nanotubes (SWNTs) that contain fullerene (C_{82}) encapsulated gadolinium ions (GdMF). As reported in the February 28 issue of *Nature*, research led by Young Kuk from Seoul National University demonstrated that bandgap energies of single SWNTs were tailored with ~3-nm accuracy using GdMF insertion to induce changes in nanotube structure and electronic environment and divide the nanotube into multiple quantum dots. Scanning tunneling microscopy (STM) was employed to monitor changes in tunneling conductivity to probe for breaks in symmetry imposed on the SWNTs. The major motivation is the development of nanoscale electronic devices as alternatives to Si-based devices.

The metallofullerene insertion into SWNTs was accomplished by heating the two in a glass ampoule at 500°C for three days. The diameters of the GdMF inserted were slightly larger than the SWNTs and could be spaced in a systematic fashion (every 1.1 nm) or quasi-periodically (every 1–3 nm), depending upon either a sonication or annealing method. The GdMF and SWNTs were both fabricated by a dc arc-discharge method, with the GdMF purified through high-performance liquid chromatography, and SWNTs purified by treatment with acid.

Using STM operated at ~5 K, dI/dV spectra were obtained from the images to estimate the bandgap at 512 points along a 10-nm section of a single SWNT. In areas that did not contain GdMF density, the SWNTs had a bandgap of 0.43 eV, while in the areas of GdMF insertion, the bandgap decreased to 0.17 eV. The evidence for such changes in tunneling conductivity along single SWNTs could be easily seen in the STM images, with bright "spots" appearing in a periodic fashion. Such bright spots are likely to be from both bandgap change and also topography change. The researchers believe insertion of GdMF into SWNTs has two effects along this line. First, the electron transfer from both the Au(111) substrate and the GdMF cluster may lead to charge transfers, resulting in the bandgap change. Second, the insertion of a GdMF with a greater diameter than the SWNTs introduces an elastic strain of the SWNTs, contributing to additional bandgap change.

The researchers believe that this ability to transform a SWNT into a one-dimensional multiple-quantum-dot system may contribute to the fields of nanoelectronics, nano-optoelectronics, and perhaps even a quantum cascade laser or quantum computer.

MATHEW M. MAYE

Computational Technique Facilitates Modeling of Fluid Transport in Porous Media

Computational materials scientist Clint Van Siclen, from the Idaho National Engineering and Environmental Laboratory, has demonstrated a theoretical approach to modeling fluid transport in porous, variable materials such as rock. Through his approach, called the walker diffusion method (WDM), Van Siclen calculates how electricity "diffuses" through a composite material. The WDM is based on the concept of a single random walker—a theoretical construct that "walks" through the material, randomly taking a step in one direction, a step in another direction, and so on. Left alone long enough, the walker will eventually explore all the potential paths available. By tracking these paths, Van Siclen is able to map out the fluid-flow routes in a permeable material, including sharp twists and turns or the tiniest of crack lines.

As reported in the February issue of *Physical Review E*, Van Siclen maps out the movements of the walker by first digitizing the structure of the porous material. That digitized representation is thus a square or cubic array of pixels or voxels, each of which is open or closed, corresponding to pore space and impermeable rock, respectively. If a pixel is open, there is a high probability that a walker will travel through that space. If the pixel is closed, then a walker will not be able to occupy that space. In a relatively short period of time, a walker can explore the accessible space using these simple, quickly computed probabilities. The calculations go even faster if several non-interacting walkers are used. These paths reveal the overall physical structure of the material.

With the conventional approach to calculating flow paths, called the finite-difference method (FDM), researchers take the digitized sample and construct a very large set of finite-difference equations, that is, equations that define the difference between the values of a function at two discrete points. Those equations have to be solved simultaneously, a task that strains the capabilities of all but the largest computers for realistically sized systems. In contrast, the WDM can be performed on a typical PC.

Furthermore, Van Siclen reports, the WDM obtains the "correlation length" for the material under study. This parameter is the size above which a specimen is uniform (homogeneous) with respect to the transport property of interest, such as fluid permeability, and below which it is variable (heterogeneous). The existence of the correlation length, which may be tens or hundreds of meters in the case of fractured bedrock, thus fundamentally limits the extent to which results from laboratory experiments are applicable to field sites.

According to Van Siclen, the WDM enables very large, or highly resolved,