Researchers take molecule's temperature

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You can touch a functioning light bulb and know right away that it's hot. Ouch! But you can't touch a single molecule and get the same feedback.

Rice University researchers say they have the next best thing -- a way to determine the temperature of a molecule or flowing electrons by using Raman spectroscopy combined with an optical antenna.

A new paper from the lab of Douglas Natelson, a Rice professor of physics and astronomy, details a technique that measures the temperature of molecules set between two gold nanowires and heated either by current applied to the wires or laser light. The paper was published this week in the online edition of *Nature Nanotechnology*.

Natelson, postdoctoral research associate Dan Ward and their colleagues found that while measuring heat at the nanoscale can be much more complicated than taking the temperature of macro objects, it can be done with a level of accuracy that will be of interest to the molecular electronics community or anyone who wants to know how heating and dissipation work at very small scales.

"When you get down to making small electronic devices or tiny junctions, you have to worry about how energy ends up in the form of heat," Natelson said. "In the case of macroscopic objects, like the filament in a light bulb, you can attach a thermocouple -- a thermometer -- and measure it." When light bulbs get hot, they also glow. "If you look at the spectrum of the light coming out, you can figure out how hot it is," he said.

That's an over-simplified version of what Natelson and Ward are doing. One can't see the glow of a molecule. However, the researchers can send in light as a probe and detect the wavelength of the light that molecule is returning when heated. "In Raman scattering, you send in light that interacts with your target. When it comes back, it will either have more energy than you put in, or the same, or less. And we can see that and figure out the effective temperature of whatever is scattering the light."

The new work follows a paper published in September about the lab's creation of nano antennas that concentrate and magnify light up to 1,000 times. That paper focused on the intensity of laser light shot into a gap between the tips of two gold nanowires.

This time, Natelson and Ward spread molecules -- either oligophenylene vinylene or 1-dodecanethiol -- on the surface of a gold nanowire and then broke the wire, leaving a nanoscale gap. When they were fortunate enough to find molecules in the gap -- "the sweet spot" being where the metal wires are closest, Natelson said -- they'd power up and read the resulting spectra.

The experiments were carried out in a vacuum with materials cooled to 80 kelvins (-315 degrees Fahrenheit). The researchers found they could easily detect temperature fluctuations of up to 20 degrees in the molecules.

On the macro level, Natelson said, "You're usually looking at something that's essentially cold. You send in light, it dumps some of the energy into the thing you're looking at and the light comes out with less energy than when you started. With Raman scattering, you can actually see particular molecular vibrational modes."

But the opposite can happen if the atoms are already vibrating with stored energy. "The light can grab some of that and come out with more energy than when it started," he explained.

The effect is most dramatic when current is supplied through the nanowires. "As we crank up the current through this junction, we can watch these different vibrations shaking more and more. We can watch this thing heat up."

Natelson, named by Discover magazine in 2008 as one of the nation's top 20 scientists under age 40, said the experiments show not only how molecules wedged into the nanogap heat up, but also their interaction with the metal wires. "The vibrations show up as sharp peaks in the spectra," he said. "They have very definite energies. Underneath all that, there's this sort of diffuse smear where the light instead is interacting with the electrons in the metal, the actual metal wires."

Natelson said it's extremely hard to get direct information about how heating and dissipation work on nano scales. "In general, you can't do it. There's a lot of modeling, but in terms of experimental things you can actually measure that tell you what's happening, everything is very indirect. This is an exception. This is special. You can see what's happening.

"In our fantasy experiment, we'd say, 'Boy, I wish I could go in with a thermometer,' or, 'I wish I could see each molecule and see how much it's shaking.' And this is effectively a way of doing that. We can really watch these things heat up."

More information: www.nature.com/nnano/journal/v … /nnano.2010.240.html

Provided by Rice University