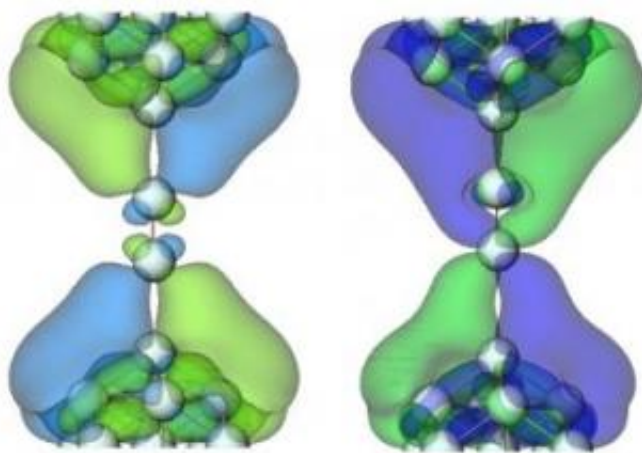


Scientists find why conductance of nanowires vary

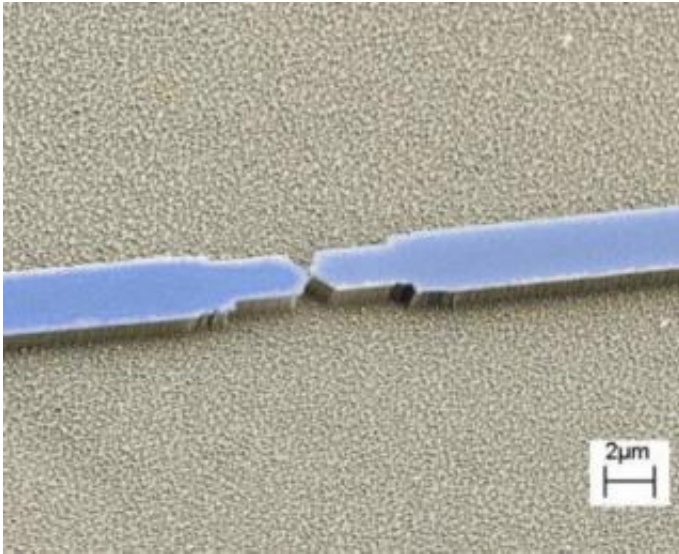
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A model of the niobium nanowire with the electrical leads on the outside and the two dimers in the center. At left, the dimer is in the center of the leads, giving it high electrical conductivity. At right, the dimer is not centered, giving it lower conductivity. For the full image click the link below. Credit: Georgia Tech/Uzi Landman

A Georgia Tech physics group has discovered how and why the electrical conductance of metal nanowires changes as their length varies. In a collaborative investigation performed by an experimental team and a theoretical physics team, the group discovered that measured fluctuations in the smallest nanowires' conductance are caused by a pair of atoms, known as a dimer, shuttling back and forth between the bulk electrical leads. Determining the structural properties of nanowires is a

big challenge facing the future construction of nanodevices and nanotechnology.



Colorized scanning electron micrograph of the device showing the two electrical leads. The nanowire connecting the tips of the leads is too small to be seen.

Credit: Georgia Tech/Alexei Marchenkov

The paper appears in the January 26th issue of *Physical Review Letters*.

"By combining the data from the electrical conductance experiments with high-level first principles quantum mechanical calculations, we've been able to draw an accurate picture of the physical mechanisms that govern these properties. It's like measuring current through an object you can't see to tell you what it looks like," said Uzi Landman, director of the Center for Computational Materials Science, Regents' and Institute professor, and Callaway chair of physics at Georgia Tech.

Leading the experimental team, Alexei Marchenkov, assistant professor

in the School of Physics, formed niobium nanowires using the mechanically controlled break junction technique – that is bending a thin nanofabricated strip of niobium until it breaks. In the final stage before the strip breaks completely, all that's left is a nanowire made of a short chain of niobium atoms that bridge the gap between the two sides of the strip. Working at low temperatures, Marchenkov was able to hold the nanowires at successive stretching stages for many hours, long enough to perform thorough conductance measurements, and much longer than the seconds typically characteristic of this technique.

Conducting the experiment at 4.2 degrees Kelvin (far below niobium's superconductivity transition temperature of 9.2 Kelvin), as well as performing measurements above the transition temperature, Marchenkov's team measured the electrical conductance of the atomic nanowire as it is stretched during the bending of the strip. As this bending occurs, the atoms separate from each other. The researchers were capable of controlling this separation with a precision better than 1 picometer (one thousandth of a nanometer), which is about 100 times smaller than the typical size of atoms.

As the nanowire is slowly pulled, the conductance drops. The drop in conductance was gradual until a rapid decrease in the conductance was observed in a narrow region of just 0.1 angstrom . Upon further pulling of the wire, the conductance resumed its gradual decline.

"Focusing on this narrow region, we found that this steep drop in conductance wasn't as smooth as it seemed at first," said Marchenkov. "We saw that the conductance actually jumps between two values. Close to the onset of the rapid drop, the conductance was mostly rather high and then there would be random short periods where it drops to a significantly lower value. On the other side of the interval, the pattern reversed itself and mostly the low conductance values were spotted with the random occurrence of sharp spikes of high conductance," said

Marchenkov.

"That's where the theoretical simulations come in," said Landman. "We needed to find out what physical phenomenon would account for these sharp drops and spikes in the conductance."

At first, the team thought a single atom must be randomly shuttling itself back and forth between two positions in the space separating the electrical leads, but the data didn't fit. So, they tried running the simulations with a connected pair of atoms, or dimer.

"When we performed electronic structure and electrical conductance calculations on a shuttling dimer, we found good agreement with the experimentally measured conductance and its variation with the wire length," said Landman.

When the dimer is closer to one lead, the electrons that make up the electrical current have a longer way to hop from the dimer to the other lead, making current flow more difficult. When the dimer is in the center between the leads, the distance the electrons have to hop is shorter and more manageable, allowing the current to flow better. As the wire bends more and more, the dimer begins to spend more of its time closer to one electrical lead than in the center, accounting for the overall decrease in conductance.

"Determining the structures of nanowires is a very big challenge in this field," said Landman. "This research shows that if you make detailed measurements and analyze them theoretically, you can determine the physical structures. In this way, measurements of electronic transport can serve not only as a probe of the electronic state of nanowires but also as a microscopy of the atomic arrangements," said Landman.

Source: Georgia Institute of Technology

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