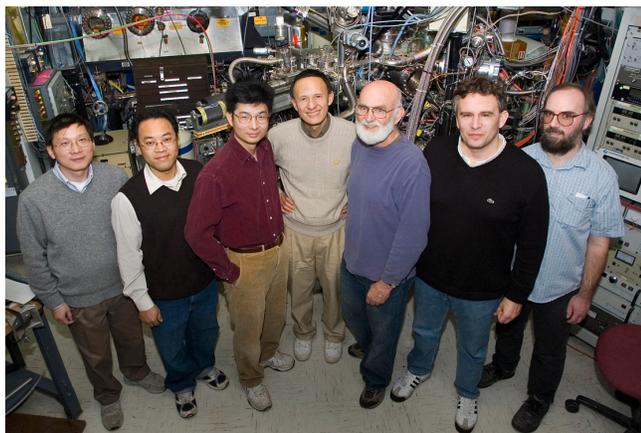


Featured Highlight

Exploring High-Dielectric Materials Through a New Route

Using integrated techniques at the NSLS and the electron microscopy facility in Brookhaven's Condensed Matter Physics and Materials Science Department, a team of researchers developed a powerful method for probing materials that could help further miniaturize microelectronic components.

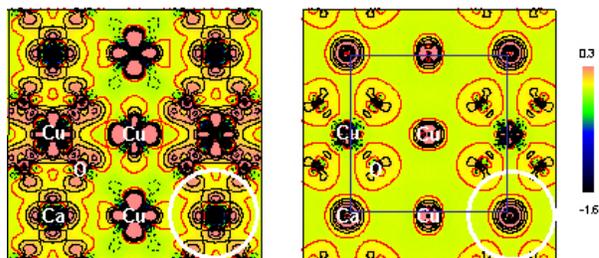
As electronic devices continue to shrink, so must components such as capacitors. However, past a certain size, the silicon-based material that's traditionally used to manufacture the critical electronic circuits starts to leak current and no longer performs as it does at larger scales. To prevent this effect, researchers have been searching for materials with high dielectric constants (or high-k), which enable the use of even smaller capacitors within the electronic world. One of the best materials for this purpose is called CCTO, which is made of calcium, copper, titanium, and oxygen.



Authors (from left) Lijun Wu, Jincheng Zheng, Wei Ku, Yimei Zhu, Jonathan Hanson, Anatoly Frenkel, and Paul Northrup

"CCTO was discovered a few years ago, but only recently it was found to have one of the highest dielectric constants ever measured," said Brookhaven physicist Yimei Zhu.

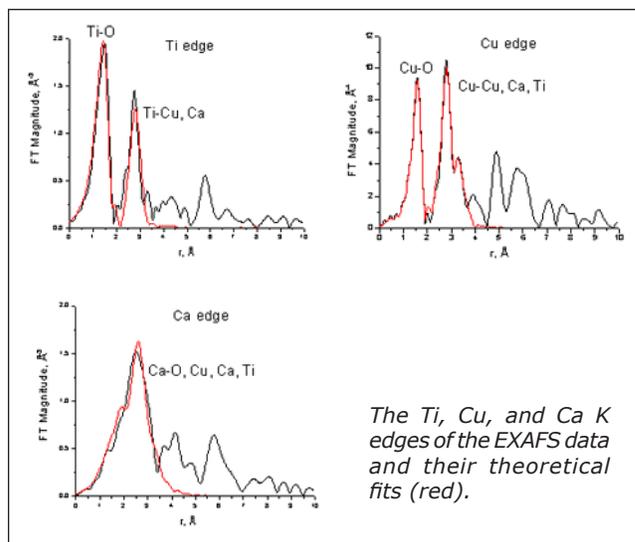
Materials with a dielectric constant greater than or equal to 7 usually qualify as high-k materials. At 100,000, the dielectric constant of CCTO far surpasses that benchmark. This intriguing property offers promising technological applications, such as the miniaturization of random access memories, as well as resonators and filters for microwave and wireless communications. There's just one problem: No one could figure out why this anomaly existed. In a recent study, Zhu's team set out to find an answer.



The bonding-electron distribution of CCTO containing Cu, Ca, and O atoms. (left) Experimental observation extracted from structure factor measurements using combined electron and x-ray diffraction data. (right) DFT calculation based on the ideal crystal structure.

First, using quantitative electron diffraction on single crystals of CCTO to measure valence electron distribution, the scientists identified broken symmetry in the electronic density of the material. They then further explored this nanoscale disorder with extended x-ray absorption fine structure (EXAFS) at NSLS beamlines X11A and X15B, as well as with theory calculations.

Specifically, the researchers found that a certain number of copper and calcium atoms switched positions within the material, which at least partially results in the high dielectric response. Their results were published in the July 20, 2007 issue of *Physical Review Letters*.



The Ti, Cu, and Ca K edges of the EXAFS data and their theoretical fits (red).

This type of nanoscale disorder was previously ignored by researchers in the field because of the lack of sufficient probing tools, Zhu said.

“Our study shows how integrated experiments can work to help solve a puzzling question and also to find a new route in searching for fascinating properties of materials –especially high-dielectric ones – by tailoring local disorder and orbital symmetry,” he said.

Other researchers involved were Jincheng Zheng, Lijun Wu, Jonathan Hanson, Paul Northrup, and Wei Ku, all from Brookhaven; and Anatoly Frenkel, from Yeshiva University. The research was funded by the Office of Basic Energy Sciences within the U.S. Department of Energy’s Office of Science.

— Kendra Snyder