Researchers Resolve 40-Year Dispute Over Disappearing Physical Property

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(PhysOrg.com) -- A property that can be used for memory in electronic devices disappears at high temperatures, and University of Arkansas scientists and colleagues in the Czech Academy of Sciences have used both theory and experiment to resolve a 40-year-old dispute over how this property disappears.

Research professor Inna Ponomareva and physics professor Laurent Bellaiche, both of the J. William Fulbright College of Arts and Sciences; Jirka Hlinka, a visiting professor from the Institute of Physics at the Czech Academy of Sciences, and their colleagues reported their findings in a recent issue of *Physical Review Letters.*

The property in question is ferroelectricity, which is found in substances that have a spontaneous polarization that can be switched by applying an electric field. These materials are used in electronic devices, but cannot be used at high temperatures, because the ferroelectric property disappears.

The researchers set out to determine why the material loses polarity – is it because the dipole moment, measured by the charge and distance between atoms, disappears completely, or is it because dipole moments become fully disordered and cancel one another? They looked at a classic ferroelectric material, barium titanate, using supercomputers to create new computational simulations and time-domain terahertz spectroscopy techniques – both cutting-edge methods for examining the issue.

“We got very good agreement between the theoretical and experimental work,” Ponomareva said.

The two scenarios depend upon the collective motion of the titanium ions, restricted by surrounding oxygen ions. Both theoretical and experimental observations show that, occasionally, whole rows of the titanium atoms make unusually large simultaneous shifts. This collective “jumping” had not been seen experimentally before.

The movement of titanium atoms helps explain the ferroelectric properties that exist in such materials, as well as why these properties disappear at high temperatures.

“These excitations had not been seen experimentally before,” said Hlinka. “Now we have a better understanding of the way this compound works.”

Bellaiche holds the Twenty-First Century Endowed Professorship in Nanotechnology and Science Education.

Citation: Coexistence of the Phonon and Relaxation Soft Modes in the Terahertz Dielectric Response of Tetragonal BaTiO3, Phys. Rev. Lett. 101, 167402 (2008)
link.aps.org/abstract/PRL/v101/e167402

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