Physicists predict Fano resonance in lead-free relaxors

November 24 2014, by Chris Branam

(Phys.org) —An international team of scientists predicts that a phenomenon known in physics as Fano resonance can exist in materials that are used in electronic devices.

The discovery advances the fundamental understanding of ferroelectric relaxors, which were discovered in the early 1960s but whose properties are still poorly understood, said Laurent Bellaiche, a Distinguished Professor of physics at the University of Arkansas.

The study was led by Dawei Wang, a former postdoctoral research associate at the University of Arkansas who is now a professor at Xi'an Jiaotong University in China. With the support of the National Science Foundation, Wang returned to the U of A as a visiting scientist to complete the two-year project.

Bellaiche and Wang study ferroelectric materials, which convert small changes in mechanical energy into electrical energy and vice versa. These changes are known as a piezoelectric response and are used in a wide range of applications that includes cell phones and heart implants.

Wang, a computational physicist, developed and used molecular dynamic computer modeling to perform accurate calculations on a certain type of relaxor, barium zirconium titanium.

The analysis of these results led to the connection between this relaxor's properties with Fano resonance, a phenomenon in which a narrow

discrete state interferes with a continuum of states.

When the discrete and continuum states don't interfere with each other, there is no resonance. In physics, resonance is the tendency of a system to vary in magnitude or position in a regular manner around a central point with greater amplitude at some frequencies than at others.

"When the states interfere," Bellaiche said, "you have something very special, which is Fano resonance. Normal relaxors are lead-based. Barium zirconium titanium exhibits these properties but is also lead-free, which is much better for applications such as cell phones."

The team published its findings on Nov. 5 in *Nature Communications*, an online journal published by the journal *Nature*, in a paper titled, "Fano resonance and dipolar relaxation in lead-free relaxors."

"This was very difficult work and provides a new perspective on the nature of lead-free relaxors," Wang said. "Determining and analyzing the dielectric response in the relaxor – how the material responds to an oscillating electric field – was the hardest part. We spent a lot of time on that."

The results were obtained through a collaborative effort with Jirka Hlinka, Petr Ondrejkovic and Jan Petzelt of the Institute of Physics in the Academy of Sciences of the Czech Republic; and Alexei A. Bokov and Zuo-Guang Ye of Simon Fraser University in British Columbia, Canada.

More information: "Fano resonance and dipolar relaxation in lead-free relaxors." *Nature Communications* 5, Article number: 5100 DOI: 10.1038/ncomms6100

Provided by University of Arkansas