Physicists determine how a promising lead-free material works

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Scientists seeking lead-free materials for use in sensors, actuators and ultrasonic motors have recently focused their efforts on a type of ceramic commonly referred to as BCZT. New research by physicists at the University of Arkansas sheds light on how this material works, providing insights that may result in other lead-free materials being developed as well.

The search for a lead-free alternative that generates a strong piezoelectrical response – the conversion of mechanical energy into electrical energy, and vice versa – at room temperature is, in part, due to restrictions on hazardous substances in electrical and electronic equipment. BCZT, an abbreviation of the chemical compound barium calcium zirconate titanate, has shown promise, but to date scientists have not fully understood why.

"In BCZT, a lead-free material, the piezoelectric response has been measured to be very large while the microscopic origin of the effect remained a matter of debate," said U of A research associate Yousra Nahas. "It became important to unveil the origin of the effect in order to better gear the properties of this material to the technological challenges."

In a paper published June 20 in the journal *Nature Communications*, U of A researchers Nahas, Alireza Akbarzadeh, Sergei Prosandeev and Raymond Walter, along with Distinguished Professor of physics Laurent Bellaiche, created an atomic-level model of the BCZT material to unlock

its piezoelectric secrets. They determined that its piezoelectric response originates from a structure that allows for easier fluctuations in polarization over a narrow temperature window around room temperature.

In addition to providing a deeper understanding of how BCZT works, the findings may point the way to creating other lead-free piezoelectric substances by mixing materials with desirable traits.

More information: Yousra Nahas et al. Microscopic origins of the large piezoelectricity of leadfree (Ba,Ca)(Zr,Ti)O3, *Nature Communications* (2017). DOI: 10.1038/ncomms15944

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