The origin of ultrahigh piezoelectric response

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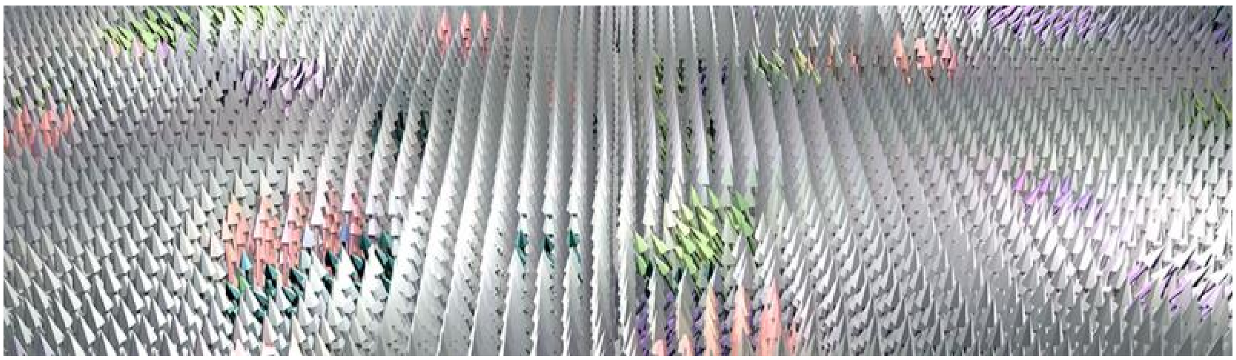

Illustration of the polar directions in relaxor-ferroelectric solid solutions where a small amount of polar nanoregions embedded in a long-range ferroelectric domain leads to dramatically enhanced piezoelectric and dielectric properties. Credit: Xiaoxing Cheng/ Penn State

All ferroelectric materials possess a property known as piezoelectricity in which an applied mechanical force can generate an electrical current and an applied electrical field can elicit a mechanical response. Ferroelectric materials are used in a wide variety of industrial applications, from ultrasound and sonar to capacitors, transducers, vibration sensors and ultrasensitive infrared cameras. Now, an international team of scientists led by Penn State may have solved the 30-year-old riddle of why certain ferroelectric crystals exhibit extremely strong piezoelectric responses.

In 1997, a relaxor-ferroelectric solid solution crystal with the highest known piezoelectric response was reported at Penn State by Thomas R. Shrout, currently senior scientist and professor of materials science and engineering at Penn State, and the late Seung-Eek Park. It has a piezoelectric response five to ten times higher than any other known ferroelectric material.

"There have been a number of mechanisms proposed to explain its ultrahigh piezoelectric responses, but none of them offer a satisfactory explanation for all the experimental observations and measurements associated with the high response. Without a firm understanding of the underlying mechanism, it would be difficult to design new materials with even higher piezoelectric response," said Fei Li, a postdoctoral scholar in materials science and engineering at Penn State and lead author of a recent article in the journal *Nature Communications* attempting to explain the phenomenon.

However, the scientific community has reached a general consensus that something called polar nanoregions contributed to the high piezo response of relaxor crystals, Li said.

A polar nanoregion is a spatial region within a crystal. It has a nanoscale size (5-10 nm) and possesses a net electric polarization. There are many such tiny regions randomly distributed in space in a relaxor crystal. Other well-known piezoelectric materials, like lead zirconate titanate (PZT), do not have polar nanoregions, but instead have much larger ferroelectric domains in which the polarization is uniform. The team set out to prove that the polar nanoregions were indeed responsible for the huge responses, and more importantly, to determine the mechanism by which they help to generate such huge responses.

The experiments were carried out at ultralow cryogenic temperatures (50-150 K). This enabled the researchers to separate the responses from the polar nanoregions, which remain active within that temperature range, from those high piezoelectric responses that typically takes place near a ferroelectric phase transition.

"We experimentally observed a significant enhancement of piezoelectric response of relaxor-ferroelectric crystals in the temperature range of 50-150 K. This enhancement accounts for 50-80% of room-temperature piezoelectricity," said Shujun Zhang, a senior author and professor of materials science and engineering at Penn State (currently at University of Wollongong).

"We attributed the experimentally observed enhancement to the existence of the polar nanoregions. Using phase-field modeling, we first proved that this significant enhancement originated from the polar nanoregions, i.e., the enhancement is absent without the presence of these polar nanoregions, and then demonstrated how the polar nanoregions help generate ultrahigh responses," said Long-Qing Chen, a senior author and Donald Hamer professor of materials science and engineering, Penn State. "Our proposed mechanism is able to successfully explain all the experimental measurements and observations associated with the high responses. This work is an important step in realizing the dream of discovering new piezoelectric materials by design.

A note of caution

"However, it should be noted that our proposed model is a mesoscale model, which is an intermediate scale. The atomistic origin of PNRs is still an open question, so further in-depth research is still required to clarify the contribution of polar nanoregions at the atomic scale. And in fact, our ongoing work is focused on understanding the atomic-scale mechanisms of polar nanoregions in piezoelectric responses," said Chen.

More information: Fei Li et al. The origin of ultrahigh piezoelectricity in relaxor-ferroelectric solid solution crystals, *Nature*

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