Smart materials used in ultrasound behave similar to water, chemists report

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Credit: George Hodan/public domain

A team of researchers at the University of Pennsylvania is gaining new insight into the smart materials used in ultrasound technology. While forming the most thorough model to date of how these materials work, they have found striking similarities with the behavior of water.

The research, published in *Nature*, was led by Andrew M. Rappe, the Blanchard Professor of Chemistry in the School of Arts & Sciences and a professor of materials science and engineering in the School of Engineering and Applied Science, and postdoc Hiroyuki Takenaka in the Department of Chemistry. Penn Research Specialist Ilya Grinberg and alumnus Shi Liu also contributed to the study.

The researchers in this group are interested in how materials interact with, harness and convert energy into different forms. In this study, they were investigating a behavior of smart material called piezoelectricity, which is the interchange of mechanical energy with electrical energy.

In piezoelectricity, applying an electric field to a material reorients dipoles within it; this is the key to the functionality of the material.

"You can imagine that there's a cage of oxygen atoms," Rappe said, "and there's a positive ion in the middle. If it sits in the middle of the cage then there's no dipole, but if it moves off-center then there's a dipole. The rearrangement of those dipoles is what leads to these smart material properties."

As the positive ions move off center, the cages of ions surrounding them either shrink or elongate in a concerted fashion, causing the material to change shape.

In ultrasound devices, providing voltage makes the material change shape, or vibrate, and those vibrations enter the human body and echo around. Piezoelectric materials are also used in sonar to allow instruments to see under water.

Recently, a set of materials was discovered that scientists believe gives higher piezoelectric performance than previous ones. But at a fundamental level, Rappe said, people didn't understand why these materials function as well as they do.

"If you don't know why it works, how could you possibly reverse engineer it and get to the next level?" he said.

Researchers often use theory and modeling to study smart materials. They have an idea of how they think a system works and can portray what an actual material is doing by solving some equations.

"One thing that we often do is solve the equations of quantum mechanics because quantum mechanics is known to be an accurate model for how electrons behave," Rappe said. "The electrons are the glue that holds the nuclei together. If you know how they're behaving, then you know what determines when bonds break and form and so forth."

But one exciting development, he said, is the ability to go beyond what researchers can afford quantum mechanically and build mechanical models to give them a more approximate way of dealing with the bonds in a solid while also allowing them to model finite temperature, larger amounts of material and for longer periods of time.

"This allows us to observe behaviors that take a long time to happen or only happen deep inside a material, and this gives us unique perspectives on complicated behaviors," Rappe said.

While other experiments have probed this material and some theoretical models have revealed certain aspects of it, the Penn researchers have now provided the most comprehensive model to date of how this material works.

Previously, scientists thought that at higher temperatures it's "every dipole for himself," making it easy for them to respond to external stimuli such as electric fields.

As the material cools down, the dipoles clump into groups called polar nanoregions. As these regions grow larger, they become sluggish and it becomes increasingly difficult for them to respond.

In this new paper, the researchers showed that, while at higher temperatures the dipoles are in fact floating free as the temperature cools and the dipoles find each other and form these polar nanoregions, the regions don't actually grow bigger but instead just become more thoroughly aligned.

This leads to the birth of domain walls within the material separating patches of different alignment. It's these domain walls between dipolar regions that lead to enhanced piezoelectric properties in the material.

This echoes a similar behavior in water, wherein the lower the temperature the more correlated the dipoles become, but the correlation doesn't hold at larger distances.

"They're never perfectly aligned," Rappe said. "Nearby water dipoles may get more and more aligned, but because of hydrogen bonding there's some intrinsic size beyond which it doesn't grow."

Piezoelectric materials are an important element in transducers, actuators and sensors used in many industries. Lack of understanding about how they work has slowed the improvement of higher quality materials. This paper provides a novel understanding of how they function and reveals similarities with the behavior of water.

A more complete understanding of why these materials behave the way they do can unlock new materials design, leading to higher quality piezoelectrics that may revolutionize smart material applications.

"It's exciting to be able to build up a model from individual electrons up to millions of atoms at finite temperature and observe complex properties," Rappe said, "and it's exciting that observing those complex properties gives us new productive directions where we can enhance materials that will more efficiently convert energy for useful devices to help people."

More information: Hiroyuki Takenaka et al, Slush-like polar structures in single-crystal relaxors, *Nature* (2017). DOI: 10.1038/nature22068

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