

# NIST pings key material in sonar, closes gap on structural mystery

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Using a neutron beam as a probe, researchers working at the National

Institute of Standards and Technology have begun to reveal the crystal structure of a compound essential to technologies ranging from sonar to computer memory. Their recent work\* provides long-sought insight into just how a widely used material of modern technology actually works.

The compound is a "piezoelectric," a material capable of changing one kind of energy into another—mechanical to electrical, or vice versa. Long employed in sonar systems to detect sound waves, more recently piezoelectrics have been applied in devices that require minuscule changes in position, such as the head that reads data from your computer's hard drive.

For decades, the industry standard piezoelectric has been PZT, a compound that contains titanium, zirconium, lead and oxygen. Crystals of PZT change a tiny fraction of a percent in size when a sound wave strikes them, and this shape change creates an electrical impulse. Decades ago, it was discovered that PZT performs at its best when the titanium and zirconium appear in approximately equal proportions, but no one really understood why.

"The theories frequently concern what happens at the transition line between having a surplus of zirconium and one of titanium," says Peter Gehring of the NIST Center for Neutron Research (NCNR). "Some theories suggest that right near the transition zone, the atoms take on a special configuration that allows certain atoms to move more freely than they can otherwise. But because it's been hard to grow a crystal of PZT large enough to analyze, we couldn't completely test these ideas."

A breakthrough came when chemists at Canada's Simon Fraser University managed to grow single crystals of a few millimeters in size and sent them to the NCNR for examination with neutron scattering—a technique for determining the positions of individual atoms in a complex [crystal structure](#) by observing the patterns made by neutrons bouncing

off it. The team, which also included researchers from the University of Oxford, the University of Tokyo, and the University of Warwick, was able to definitively rule out one of the proposed structures of PZT.

Instead, they found that each PZT crystal element likely assumes one of two possible forms that coexist within the larger crystal array. These forms are dictated by chemical composition, and they may influence how well the material performs on a large scale. Their findings also suggest that the change in behavior seen at the transition happens gradually, rather than at some sharply delineated proportion of zirconium to titanium.

Gehring says the results could be a step toward bettering PZT.

"Determining the structure might give us the perspective necessary to design a piezoelectric material from first principles, instead of just playing around and seeing what works," he says. "That's what you need if you're ever going to build a better mousetrap."

**More information:** \* D. Phelan, X. Long, Y. Xie, Z.-G. Ye, A.M. Glazer, H. Yokota, P.A. Thomas and P.M. Gehring. Single crystal study of competing rhombohedral and monoclinic order in lead zirconate titanate. *Physical Review Letters*, Nov. 8, 2010, [DOI:10.1103/PhysRevLett.105.207601](https://doi.org/10.1103/PhysRevLett.105.207601)

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