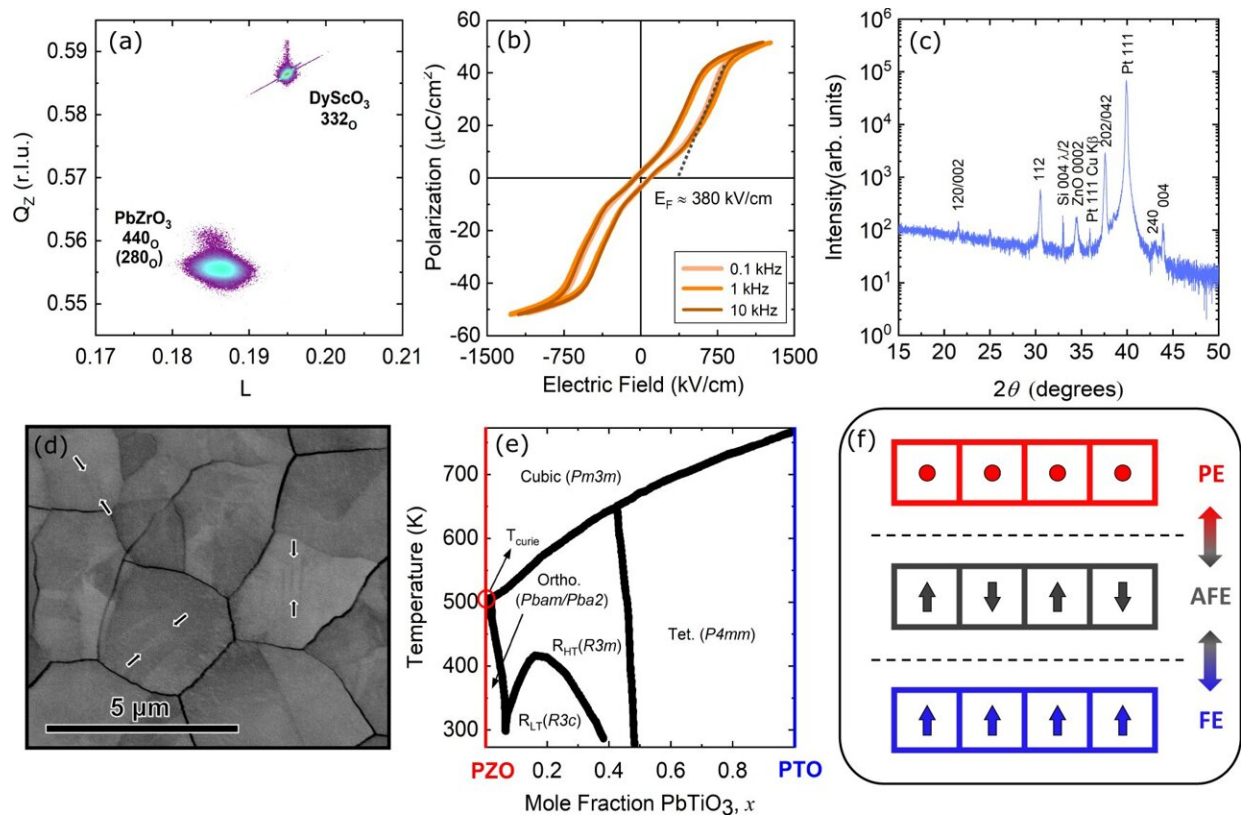


Researchers harness the power of a new solid-state thermal technology

June 21 2022, by Karen Walker



Structural phase transformations in PZO upon electrical and thermal stimuli. a) Reciprocal space map of the PbZrO₃ 440/280 and DyScO₃ 332 reflections demonstrating epitaxial growth and the presence of ferroelastic domains in the epitaxial film. b) Polarization-electric field hysteresis response for the epitaxial PbZrO₃ film showing antiferroelectric switching. c) 2θ-ω XRD pattern for the polycrystalline PbZrO₃ film. d) Channeling-contrast backscatter electron micrograph of the polycrystalline PbZrO₃ film. The arrows indicate the locations of clearly resolved ferroelastic domains. e) Phase diagram for lead

zirconate titanate ($\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$, PZT) recreated from ref. 27. f) Schematic of dipole orientation across antiferroelectric to ferroelectric (AFE-to-FE) and antiferroelectric to paraelectric (AFE-to-PE) phase transitions. Credit: Kiumars Aryana et al, *Nature Communications* (2022). DOI: 10.1038/s41467-022-29023-y

Researchers at the University of Virginia School of Engineering and Applied Science have discovered a way to make a versatile thermal conductor, with promise for more energy-efficient electronic devices, green buildings and space exploration.

They have demonstrated that a known material used in electronic equipment can now be used as a thermal regulator, too, when it is in a very pure form. This new class of material gives engineers the ability to make [thermal conductivity](#) increase or decrease on demand, changing a thermal insulator into a conductor and vice versa.

The team published its findings earlier this spring in *Nature Communications*. The paper is titled "Observation of Solid-state Bidirectional Thermal Conductivity Switching in Antiferroelectric Lead Zirconate."

Bi-directional control or "tuning" of thermal conducting materials will be especially useful in electronics and devices that need to operate in [extreme temperatures](#) or withstand extreme temperature fluctuations. One of the scenarios where devices need to perform under such harsh conditions is space.

"The temperature fluctuations in space can be pretty intense," said Kiumars Aryana, who earned his Ph.D. in mechanical and aerospace engineering at UVA this spring and is first author of the *Nature Communications* paper. "This type of thermal transport technology could

be a huge advantage as we build vehicles and devices for space exploration."

"The Mars rover is a great example," Aryana said. Ground temperatures at the rover landing sites can reach 70 degrees Fahrenheit during the day and minus 146 degrees at night. To keep electronic devices working through these wide temperature swings, the rover relies on an insulating box and heaters to keep the components from freezing and radiators to prevent them from burning up.

"This new mode of heat management is substantially less complex and means heat regulation is easier to manage—and faster. Where a radiator or insulation takes a long time to start heating or cooling, the solid-state mechanism would be almost instantaneous. Being able to keep up with the rapid temperature changes also makes things safer. Because the heating and cooling can keep up, the chances of the heat or cold causing malfunctions—or worse—are decreased," Aryana said.

Meanwhile, here on Earth, promising uses include managing heating and cooling on a large scale, like buildings, and a small scale, like circuit boards for electronics. Less energy equates to greener technology and lower costs.

This advancement continues a longstanding collaboration between Jon Ihlefeld, UVA Engineering's associate professor of materials science and engineering, and electrical and computer engineering, and Patrick E. Hopkins, Whitney Stone Professor of Engineering and professor of mechanical and aerospace engineering and Aryana's advisor.

The Ihlefeld-Hopkins team has pioneered tunable thermal [conductivity](#) in crystalline materials over the course of a decade, first at Sandia National Laboratories and now at UVA.

Tunability is unique to a class of functional materials called ferroelectrics, a specialty of Ihlefeld's multifunctional thin-film research group.

"A ferroelectric material is like a magnet, except instead of a north and south pole, you have a positive and negative charge," Ihlefeld said. An [electric field](#), or voltage, when applied to a ferroelectric material, "flips" the polarity of the material's surface to its opposite state, where it remains until an opposite voltage is applied.

"Usually, thermal conductivity is considered a static material property," Hopkins said. "If you want to change a [thermal conductor](#) into an insulator, you have to permanently change its structure or integrate it with a new material."

Ihlefeld's and Hopkins's prior research demonstrated how to lower thermal conductivity with an electric field, and how to integrate the material within a device to make thermal conductivity rise, but they could not make the same material do both.

For this project, the team used an antiferroelectric material in which heat and voltage both come into play.

"What this interesting material does, in addition to being a high-quality crystal that has thermal conductivity trends like an amorphous glass, in addition to being solid-state, is it gives us two unique knobs to change thermal conductivity," Hopkins said. "We can rapidly heat the crystal with a laser or apply voltage to actively tune thermal conductivity and heat transport."

"We tried to use a commercial sample of [lead zirconate](#) for testing bi-directional thermal conductivity, but it didn't work," Aryana said. Lane Martin, Chancellor's Professor of Materials Science and Engineering and

department chair at the University of California Berkeley, provided an extremely pure sample of lead zirconate. "Using Lane's sample, we achieved a 38% bi-directional change in thermal conductivity in one burst, which is a huge leap," Aryana said.

Antiferroelectric material structures are bi-directional by nature. In the smallest repeat unit of the crystal lattice, one half has a polarity pointing up and the other half points down, such that the positive and negative charges cancel each other out. When heated, the crystal structure changes and the antiferroelectricity goes away, increasing thermal conductivity. Applying an electric field does the opposite—it causes the material to transform into a ferroelectric and the thermal conductivity decreases. The net polarity returns to zero when the voltage is removed.

The flip in polarity and the arrangement of atoms in the crystal that support the antiferroelectric structure leads to observable and measurable thermal scattering events—something like a heat signature—which means energy diffuses through the material in ways that can be predicted and controlled.

Members of Hopkins's experiments and simulations in thermal engineering research group have made many advances in laser measurement of materials. The *Nature Communications* paper presents an innovation in optical thermometry-based experiments in which students employed a third laser to bring about a rapid heating event to modulate the antiferroelectric film through the transition from the antiferroelectric to paraelectric structure, giving it the ability to become polarized under an applied electric field.

To make an impact on technologies, engineers will need a bigger "on-off" switch to rapidly move or store a much larger percentage of heat. The next steps for the research team include working to better define the material's limitations, so they can design a new material with higher

switching ratios, accelerating the use of actively tunable thermal conductivity materials.

More information: Kiumars Aryana et al, Observation of solid-state bidirectional thermal conductivity switching in antiferroelectric lead zirconate (PbZrO_3), *Nature Communications* (2022). [DOI: 10.1038/s41467-022-29023-y](https://doi.org/10.1038/s41467-022-29023-y)

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