Microscope reveals the secrets of a material's structure

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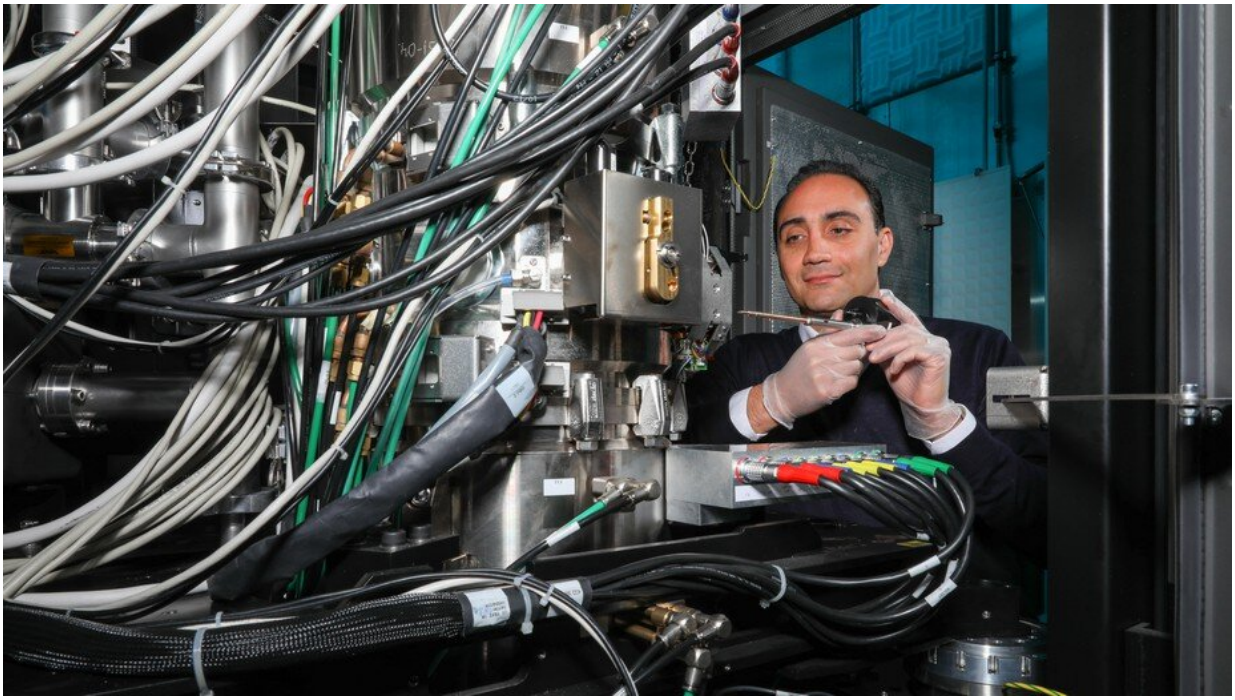


Emad Oveisi in front of the Titan-Themis microscope. Credit: Alain Herzog / 2021 EPFL

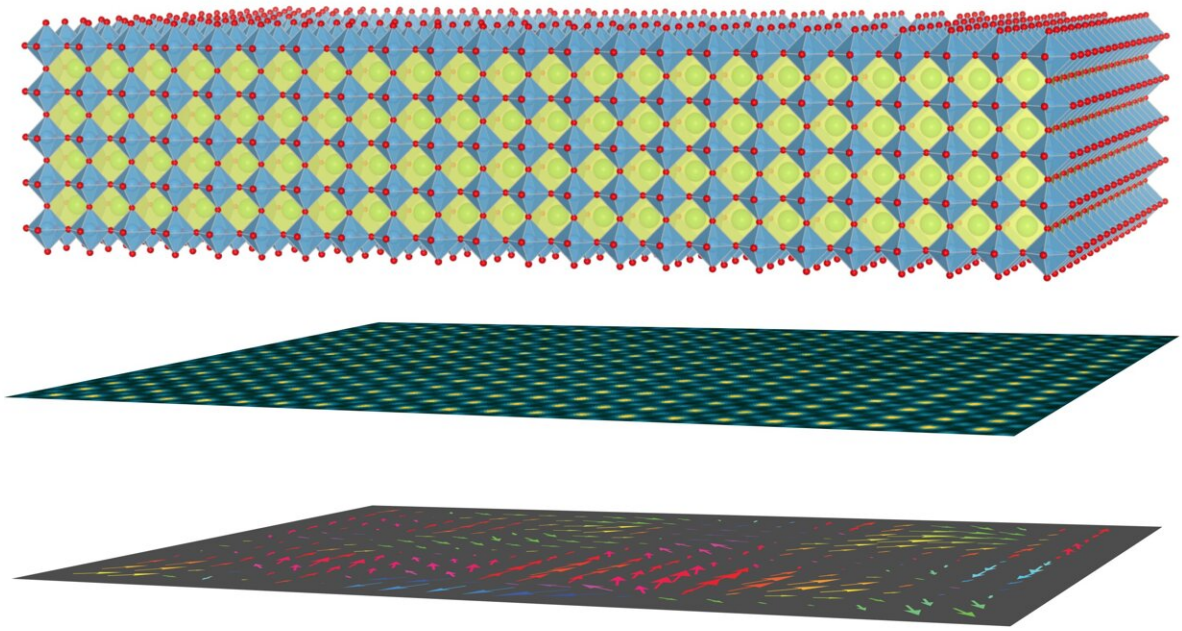
EPFL scientists have made an important discovery about the structure of barium titanate, a material used in everyday objects. Their findings refute existing theories on the displacement of the material's atoms.

Barium titanate is a ferroelectric material used in nearly all electronic

devices—computers, smartphones and even electric cars. It's used to make the sensors and capacitors they run on, for example. "A single smartphone generally has around 700 capacitors containing barium titanate, and trillions of these capacitors are made every year," says Dragan Damjanovic, an EPFL professor and head of the Group for Ferroelectrics and Functional Oxides at EPFL's School of Engineering. Despite barium titanate's widespread use, however, researchers still don't fully understand how it works. "There are of course theoretical models out there, but some of their key predictions have never been experimentally confirmed. So that's what we set out to do," says Damjanovic.

One of the world's most powerful microscopes

Emad Oveisi, a senior scientist at EPFL's Interdisciplinary Center for Electron Microscopy, suggested that Damjanovic and his Ph.D. student Sina Hashemizadeh use his center's Titan Themis—one of the world's most powerful electron microscopes—for their research. The Titan Themis enabled the scientists to observe theatomic structures of barium titanate and barium-strontium titanate in the cubic phase. That was back in 2015, when they obtained the first images; it took another five years to analyze and verify their results. "Until now, researchers believed that the atoms move in several directions in a very short timeframe. But our experiments showed that they tend to prefer certain directions, meaning there are nanometric-sized areas where all theatoms move in the same way. That completely changes how we view these materials and their atomic structure," says Oveisi. Since their findings contradicted current thinking, the scientists wanted to make sure they were right. So they tested and checked their results several times, including with peers in Slovenia, Austria and Japan. That's why it took five years to finalize the results. The study has now been published in *Nature Communications*.



The atomic structure of barium titanate. Credit: EPFL

Small-scale phenomena with large-scale repercussions

Thanks to the advanced image analaysis methods, the scientists were able to identify where in the material the atoms move in an orderly fashion. "When we talk about movements, we're actually referring to displacements that take place on a picometer scale—that is, one order of magnitude smaller than the atoms themselves," says Oveisi. Damjanovic adds: "Even though the displacements are extremely small, they have repercussions on a much larger scale. For instance, if we expose the nanometric areas we identified to a high-frequency electric field like those in smartphones, the areas heat up." His team's findings could therefore be extremely useful in better understanding energy loss in these kinds of materials.

So what's the next step? "The research is never-ending!" says Damjanovic. "The question of whether the nanometric displacement really does play a role in heating the material needs to be tested. And if it does, the next step will be to develop materials where the size of the displacement area is minimized in order to enhance the material's properties."

More information: Andreja Bencan et al, Atomic scale symmetry and polar nanoclusters in the paraelectric phase of ferroelectric materials, *Nature Communications* (2021). DOI: 10.1038/s41467-021-23600-3

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