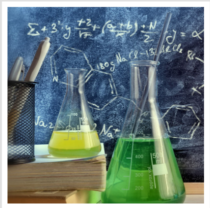
Nano Science, Technology and Industry Scoreboard

Team Demonstrates Rare Form of Ferroelectricity in Ultra-thin Material



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The nanoscopic equivalent of stacking a deck of cards — layering materials a mere few atoms thick atop one another — has emerged as a favorite pastime of material scientists and electrical engineers worldwide.

Just as cards can differ by suit and value, the properties of those atomically thin 2D materials can vary, too: electronically, magnetically, optically or in any number of other ways. And much like combining the right cards can yield valuable hands, the right combinations of 2D materials can yield technologically valuable outcomes.

The University of Nebraska–Lincoln's Alexei Gruverman, Alex Sinitskii and colleagues have now demonstrated that one particular 2D material, already considered a face card, actually ranks as an ace in the hole.

That material is molybdenum disulfide, or MoS_2. Alongside partners from Luxembourg, China and France, the Husker researchers have shown that MoS_2 possesses a long-theorized property that could help computers, phones and other microelectronics save both power and their exact electrical states, even after being turned off.

A side-view rendering of molybdenum disulfide, a technologically appealing material that consists of two sulfur atoms (yellow and green) for every one molybdenum (purple and blue). Nebraska researchers found that the upward shift of the green sulfur atoms contributes to the emergence of ferroelectricity, a prized but rare property that can help encode digital data using substantially less power.

MoS2’s power-saving, state-saving promise comes courtesy of a prized but uncommon property known as ferroelectricity. The vertical separation and arrangement of negative vs. positive charges in ferroelectric materials can be instantaneously flipped just by applying some voltage. Those oppositely aligned, or polarized, states can be read or stored as the 1s and 0s of binary data, with the states remaining even when a power source has been cut.

That set-it-and-forget-it advantage is compounded by the fact that voltage can flip polarization, and encode a respective 1 or 0, while drawing far less energy than the magnetic fields often used to encode digital data. Collectively, those benefits have positioned ferroelectric materials as a prominent player in a future even more dependent on microelectronics.

Theory-backed simulations had suggested that MoS2 was just such a material. As with other 2D materials, though, proving it had proven fiendishly difficult. But by prodding flakes of molybdenum disulfide with a nanoscopic needle that simultaneously excited the material with an electric field, the Husker-led team has managed to confirm that MoS2 is, in fact, ferroelectric. The material’s polarized states held for up to weeks at a time, the researchers said, and were observed with the MoS2 flakes sitting atop any one of several other materials.

“Ferroelectricity in two-dimensional materials is, in general, a new phenomenon,” said Sinitskii, professor of chemistry at Nebraska. “It was discovered fairly recently, and the examples of two-dimensional systems that exhibit ferroelectric polarization are still very limited.”

Ferroelectricity alone, then, would be enough to vault molybdenum disulfide up the rankings of 2D materials. Yet MoS2 features other properties that appeal to the engineers tasked with building better devices. It’s relatively easy to grow, first in bulk, then by peeling off atomically thin layers with the aid of Scotch tape. Unlike many of its 2D counterparts, it holds up when exposed to air and plays well with the oxygen-rich materials found in many electronic components.

Beyond all that, it’s a semiconducting material in the vein of silicon — the longstanding choice for integrated circuits, or microchips — meaning that its flow of electric current can be triggered and halted with minimal effort. That sets MoS2 apart from most ferroelectrics, Gruverman said.

In the wake of the team’s study, which appeared in the journal npj 2D Materials and Applications, MoS2 now joins just a handful of materials that boast high-yet-controllable conductivity and easily switchable polarization, the researchers said.

“There was always this striving to combine semiconducting and ferroelectric properties in one material, because that would make it a very powerful material — a holy grail, if you will — for the semiconductor industry,” said Gruverman, Charles Mach University Professor of physics and astronomy.

‘The structure that we observed was clearly unprecedented’

The atoms of a material can take on different configurations that generate different properties. The most famous example of the phenomenon might be carbon, which can range from a soft black lump of coal to a nigh-indestructible, transparent diamond.

Molybdenum disulfide, which consists of one molybdenum atom for every two sulfur, is no exception. In its most stable state, known as 2H, the material acts as a semiconductor yet actually lacks ferroelectricity. But prodding the MoS2 with a minuscule point shifted some of the sulfur atoms upward, the team found, altering the distances between those atoms and the molybdenum. That, in turn, altered the distribution of the atoms’ electron clouds, ultimately transforming the semiconducting 2H into a more conductive, ferroelectric phase known as 1T”.

A top-down rendering of molybdenum disulfide’s atomic structure in its 1T” configuration, with triangular groupings of purple molybdenum atoms shifting closer to the green, upward-displaced sulfur atoms. (The blue molybdenum atoms and yellow sulfur atoms are relatively undisturbed.)

To switch the polarization of MoS2, the researchers exploited the so-called flexo-electric effect: a change in the electrical behavior of a material when it begins straining under the force of a mechanical stress. For more than a half-century, physicists have known that the more variable the strain — that is, the greater the disparities in how various areas of a material will deform under stress — the more pronounced the electric polarization will be. Thicker materials tend to experience fairly uniform strains, Gruverman said, resulting in limited polarization and usefulness for encoding binary data.

A 2D material such as MoS2 — especially one pricked with the finest of fine points — is a much different prospect, yielding a huge disparity in strains and, consequently, a massive flexo-electric effect.

“In materials as thin as MoS2, this flexo-electric effect is very profound,” Gruverman said. “What’s important is that this approach could be used as a very effective tool to control polarization states in ferroelectrics.

“Now we’ve demonstrated that, in addition to the electric field, we can use mechanical stress as a way of controlling or tuning the electronic properties of these heterostructures.”

The team also discovered a surprise that could work in MoS2’s favor. Though the flakes that Sinitskii and his colleagues fabricated were virtually pristine, the team occasionally encountered polarization signals that were substantially weaker than they expected. Curious, Sinitskii had the idea to flip the flakes over and measure the signals again, hoping to glean insights on the ultra-thin third dimension of the essentially 2D material.

When they did, the researchers determined that the flakes contained randomly alternating layers of polarization — some with positive charges at the top and negative charges at the bottom, others vice versa.

“The structure that we observed was clearly unprecedented, because none of the two-dimensional ferroelectric structures that people observed before exhibited this kind of arrangement of ferroelectric domains,” Sinitskii said.

The existence of those randomly alternating layers implied another surprise. In some cases, like-signed charges are butting up against one another — positive to positive or negative to negative — without repelling each other, as they would normally be expected to. How? The team suspects that the especially high conductivity of 1T” MoS_2 promotes the flow of enough charges between those layers to prevent the repulsion. It’s possible, Gruverman said, that the intra-layer currents could be controlled by flipping the polarization of the MoS_2 flakes, offering another, hyper-localized way to encode data.

“It’s quite unusual to have these layers of a material where polarization in one layer doesn’t care about the polarization state in the adjacent layer,” Gruverman said. “Usually, this kind of head-to-head and tail-to-tail configuration would be very unfavorable. Yet it seems that, here, these layers are absolutely non-sensitive to the polarization state in the neighboring layers.”

But the full promise of molybdenum disulfide may only reveal itself, Sinitskii said, when material scientists — now knowing the true value of MoS_2 — manage to play it in just the right hands.

“This is a very hot topic right now,” Sinitskii said. “There are many people who are really shuffling these different layers and stacking them on top of each other. Now they have another kind of two-dimensional material that could be added to those stacks and make them more diverse, more programmable and, eventually, more useful.”

Read the original article on University of Nebraska Lincoln.