Under pressure, 'squishy' compound reacts in remarkable ways

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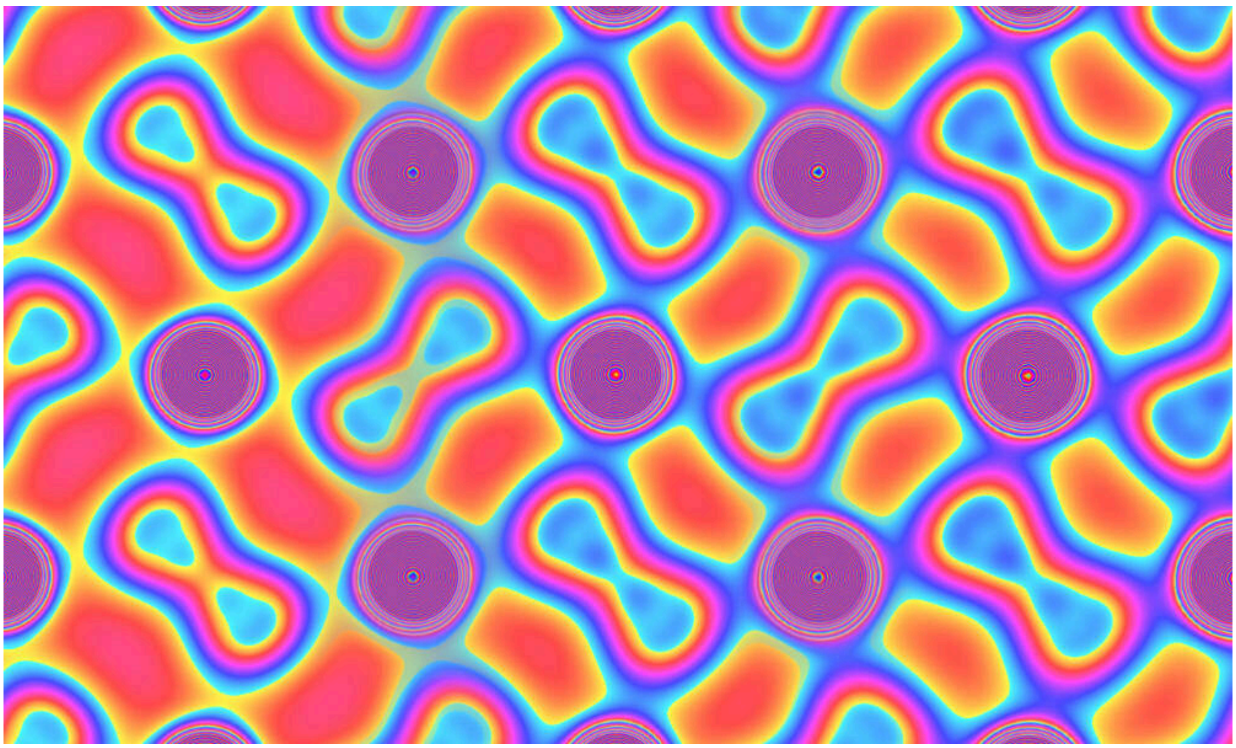

As a compound of manganese sulfide is compressed in a diamond anvil cell, it undergoes dramatic transitions. In this illustration, the interaction between the manganese (Mn) atomic ions (purple circles) and disulfur (S_2) molecular ions (figure 8s) increases from left to right until the overlap is significant enough to make the system metallic. Credit: Dean Smith, Argonne National Lab

Remarkable things happen when a "squishy" compound of manganese and sulfide (MnS_2) is compressed in a diamond anvil, say researchers from the University of Rochester and the University of Nevada, Las Vegas (UNLV).

"This is a new type of charge transfer mechanism, and so from a science community point of view this is very, very exciting. We are showing remarkable physical transformations over a very, very short range of parameters, in this case pressure," says Ashkan Salamat, associate professor of physics at UNLV.

For example, as the pressure increases, MnS_2, a soft insulator, transitions into a metallic state and then into an insulator again, the researchers describe in a paper flagged as an editor's choice in *Physical Review Letters*.

"Metals usually remain metals; it is highly unlikely that they can then be changed back to an insulator," says Ranga Dias, assistant professor of mechanical engineering and of physics and astronomy at Rochester. "The fact that this material goes from an insulator to a metal and back to an insulator is very rare."

Moreover, the transitions are accompanied by unprecedented decreases in resistance and volume across an extremely narrow range of pressure change—all occurring at about 80 degrees Fahrenheit. The relatively low temperature enhances the chances that the metal transition process might eventually be harnessed for technology, Salamat says.

In previous papers in *Nature* and *Physical Review Letters*, the Dias and Salamat collaboration set new benchmarks toward achieving superconductivity at room temperatures. A common denominator of their work is exploring the "remarkably bizarre" ways transition metals and other materials behave when they are paired with sulfides, and then compressed in a diamond cell anvil.

"The new phenomena we are reporting is a fundamental example of responses under high pressure—and will find a place in physics textbooks," Salamat says. "There's something very intriguing about how sulfur behaves when it is attached to other elements. This has led to some remarkable breakthroughs."

The breakthroughs achieved by the Dias and Salamat labs have involved compressing mere picoliters of material—about the size of a single inkjet particle.

Spin and pressure underlie dramatic metal transition

Underlying the transitions described in this paper are the way the spin states (angular momentum) of individual electrons interact as pressure is applied, Dias and Salamat explain.

Bizarre things can happen when transition metals and other materials are compressed in a diamond anvil. Here, Ranga Dias holds an array containing diamond anvil cells. Credit: University of Rochester photo / J. Adam Fenster

When MnS_2 is in its normal insulator state, electrons are primarily in unpaired, "high spin" orbitals, causing atoms to actively bounce back and forth. This results in the material having higher resistance to an electrical charge because there is less free space for individual electrons trying to pass through the material.

But as pressure is applied—and the material is compressed toward a metallic state—the electron orbitals "start to see each other, immediately come toward each other, and pairs of electrons start linking up as one," Salamat says.

This opens up more space for individual electrons to move through the material—so much so that resistance drops dramatically by 8 orders of magnitude, as pressure is increased from 3 gigapascals (435,000 psi) to 10 gigapascals. This is a relative "nudge" compared to the 182 to 268 gigapascals required for superconducting materials.

"Given the small range of pressure involved, a drop in resistance of this magnitude is really enormous," Dias says.

Low resistance is maintained even in the final phase—when the MnS_2 reverts to an insulator—because the electrons remain in a "low spin" state.

Basic materials science, future technological advances

As often occurs with new discoveries in basic science, the possible applications have yet to be explored.

However, Salamat says, a transition metal which, with a relatively small amount of strain, can jump from one state to another—at room temperature, no less—is likely to be useful.

"You could imagine having a logic switch or writing hard disk, where a very, very small permutation in strain or voltage could make something jump from one electronic state to another. New versions of flash memory, or solid state memory, could permutate and take on a new approach using these types of materials," Salamat says.

"You can do quite aggressive maneuvers to drive these materials at 300 kelvin, making them potentially useful for technology."

Lead author Dylan Durkee, a former undergraduate researcher in the Salamat lab, is now working as a graduate student with Dias. Other coauthors include Nathan Dasenbrock-Gammon and Elliot Snider at Rochester; Keith Lawler, Alexander Smith, and Christian Childs at UNLV; Dean Smith at Argonne National Laboratory, and Simon A.J. Kinder at University of Bourgogne.

More information: Dylan Durkee et al, Colossal Density-Driven Resistance Response in the Negative Charge Transfer Insulator MnS_2, *Physical Review Letters* (2021). DOI: 10.1103/PhysRevLett.127.016401

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