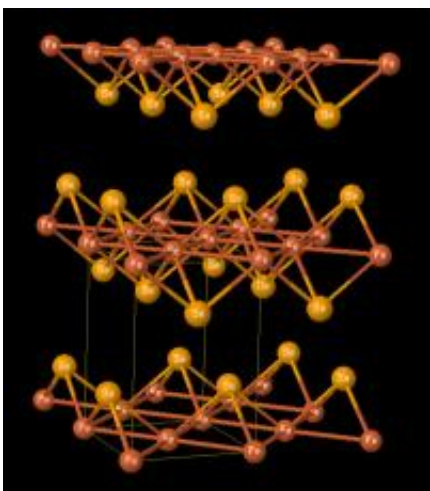


Watching the Tug of War between Structure and Superconductivity

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The crystalline structure of the superconductor FeSe has square layers of iron (Fe) atoms that are strongly chemically bonded to layers of selenium (Se) atoms. The superconducting electrons are found in the iron layers. The group's work showed that a deviation of the shape of the iron layers from exactly square geometry at the length scale of thousands of atoms is a critical factor in determining whether superconductivity occurs or doesn't occur.

(PhysOrg.com) -- Like Clark Kent, who often forgoes his social life to become Superman, materials that become superconducting must sacrifice at least one of their natural properties to attain the ability to transfer electric current with zero resistance. At the NSLS and Brookhaven's Center for Functional Nanomaterials (CFN), a team of researchers has explored this internal conflict in a class of iron-based

superconductors, materials that could be used to develop energy-saving applications such as high-efficient power lines.

Relatively new to the field of superconductivity, iron-based materials are now world-famous for their frictionless transport of electrons at "high" temperatures — above about 50 Kelvin, or -190 degrees Celsius.

"Iron-based superconductors have second highest [transition temperature](#) that anyone knows about, a characteristic that's very important if we want to use them for practical applications," said Princeton researcher Robert Cava. "All aspects of research on these materials are now underway. Our part of the picture is to try and understand why they're superconducting in the first place."

Cava and a group of fellow researchers from Princeton, Stony Brook University, Brookhaven, and Johannes Gutenberg University, in Germany, focused their investigations on a particular material made from conducting layers of iron and selenium, called iron [selenide](#). In recent years, scientists have explored numerous aspects of the underlying physics of iron-based superconductors, often making connections to the material's structure or innate magnetism. But the exact relationships between these properties were unclear.

"In order for superconductivity to exist, it must arise as the winner in a tug of war between different physical properties," Cava said. "The research community has known that magnetism competes with superconductivity in the iron [superconductors](#), but no one had a good idea of how crystal structure competed."

Cava's group compared the structures of superconducting and non-superconducting iron selenide using two different types of tools: powerful beams of x-rays at the NSLS and a suite of advanced microscopes at the CFN. At NSLS beamline X16C, the researchers used

synchrotron x-ray powder diffraction to provide "snapshots" of the materials on the order of hundreds of nanometers. They combined that data with images taken with transmission electron microscopy and electron diffraction, resulting in resolution an order of magnitude higher than the x-ray technique.

"We needed both of these sophisticated techniques to really understand what was going on here," Cava said, adding that the findings weren't as straightforward as expected.

Among the results, which were published in the July 31, 2009 edition of *Physical Review Letters*, the group showed that the superconducting form of iron selenide can be distinguished from the non-superconducting form by a change in its structure. The superconductor gains its power by giving way to a slight structural "distortion," and the non-superconductor holds strong.

The researchers also showed that this unique structural change is unrelated to magnetism, as hypothesized in the past. The material's fundamental bonding — the bonding between atoms — stays the same while the angles between the bonds change, similar to the expansion of a baby gate. Unlike a gate, the angles only change by a few degrees — still enough, though, to give birth to superconductivity.

But the real surprise is that this structural change actually exists in both the superconducting and non-superconducting forms of the material, just on different scales and with different effects.

"This distortion can still be found in the non-superconducting material, but it's only present over tens of atoms," Cava said. "In the superconducting material, it's present over very long distances. This detail was hidden until we were able to take a really close look at the materials. The challenge now is to figure out over what distance a [crystal](#)

[structure](#) has to be distorted in order to affect its properties."

Next, Cava's group will try to resolve the structure-superconductivity relationships within other iron-based [materials](#).

"By showing the scientific community this clear example, we hope to inspire them to think about manipulating this phase transition," he said.

More information: T.M. McQueen, A.J. Williams, P.W. Stephens, J. Tao, Y. Zhu, V. Ksenofontov, F. Casper, C. Felser, R.J. Cava, "Tetragonal-to-Orthorhombic Structural Phase Transition at 90 K in the Superconductor Fe_{1.01}Se," PRL, 103, 057002 (2009).

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