Metal in chains

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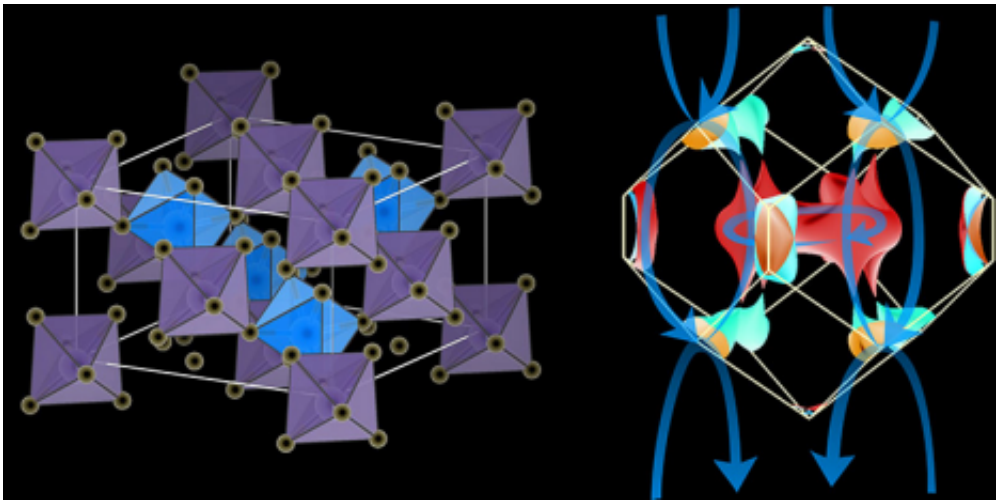

Crystal structure (left) and part of the band structure (right) of iridium tetrafluoride. The particular symmetry of the crystal lattice leads to the nodal chains (blue) in the band structure. Credit: from Bzdusek et al. *Nature*, 2016

The electronic energy states allowed by quantum mechanics determine whether a solid is an insulator or whether it conducts electric current as a metal. Researchers at ETH have now theoretically predicted a novel material whose energy states exhibit a hitherto unknown peculiarity.

If one looked deep into three different solids using a super-microscope, one would, in principle, always see the same thing: atomic nuclei arranged in a crystal lattice and electrons, of which some orbit the atomic nuclei and others criss-cross the entire crystal lattice. Nevertheless, those three materials might behave very differently when

an electric voltage is applied to them.

The first solid might, for instance, conduct an electric current, the second one might turn out to be an insulator, and the third one could be a semiconductor - that is, a material whose electric conductivity increases with increasing temperature (rather than diminishing, which is the case for metals) and that is the basis for transistors and computer chips.

A team of physicists led by Manfred Sigrist, Alexey Soluyanov and Andreas Rüegg at the Institute for Theoretical Physics of the ETH in Zurich have now predicted a new kind of solid they call "nodal chain metal" that is expected to have hitherto unknown properties. Moreover, they have already identified a potential candidate among existing materials.

Band structure and Fermi level

Two quantities determine, by and large, if and how a solid conducts electric current: its band structure and its Fermi level. The band structure refers to the possible energy states the electrons inside it can occupy. Whereas a free electron accumulates kinetic energy as it moves faster and faster, electrons embedded in a crystal lattice can only take on energy values that lie inside certain intervals or "bands".

This follows from their quantum mechanical wave nature, which is also responsible for the fact that some values of the motional energy are off limits for electrons; those are also called band gaps. The Fermi level, on the other hand, derives from the fermionic nature of electrons, which means that two of them can never occupy the same energy state. If one were to build up a solid one particle at a time, each newly added electron would try to occupy higher and higher energy levels, starting from zero energy. The energy of the last electron would then be the Fermi level.

Whether a material is a metal or an insulator can now be easily predicted if its energy bands and its Fermi level are known. If the Fermi level lies inside a band, the most energetic electrons can move easily and hence conduct electric current. If, on the other hand, the Fermi level coincides with a band gap, one has an insulator. By the same token, other materials may be metals by that definition, but with very few possible energy states at the Fermi level. "The material we predict is, if you will, a cousin of such so-called semimetals", explains Tomàš Bzdušek, a PhD student with Sigrist and Rüegg.

Nodes in the semimetal

One semimetal that has made the headlines is graphene. The particular way in which the energy bands of graphene's electrons approach each other at so-called Dirac points is responsible for the electrical and thermal conductivities of this peculiar material, whose discoverers were awarded the Nobel Prize in Physics in 2010. Since the band gap actually vanishes at the Dirac points, they are also called nodes (in analogy with the nodes of a standing wave).

In other semimetals the energy bands touch not at isolated points but along well-defined lines or surfaces. "The peculiarity of our new material is that its energy bands touch along interconnected nodal loops, and those nodal loops form a chain", says Soluyanov. "That may sound strange and rather theoretical, but we have actually found a real material that is likely to have those properties. That such nodal chains should appear is not an accident, but dictated by the symmetries of the material's crystal lattice."

Incidentally, physicists are able to draw an interesting analogy between solid state and high energy particle physics. In high-energy theories nodal chains would be impossible due to the high level of symmetry of the vacuum. In a crystal, by contrast, there are far fewer symmetries,

creating a kind of novel vacuum.

To find the nodal chain material the researchers took a long and winding road. Assuming it would be easier, they first set out to look for materials with a single nodal loop and determined what kind of symmetry properties the crystal lattice of such a material should have. All in all, 230 different types of crystal symmetries are known, and it is those symmetries that are largely responsible for the properties of a material's band structure.

Soluyanov and his colleagues then scoured massive online databases (ICSD - Inorganic Crystal Structure Database) in which thousands of known solids are listed alongside their crystal structures. Eventually, they chanced upon one that had not only a nodal loop, but the more intricate nodal chain: iridium tetrafluoride. "It was an unexpected surprise", admits Quan Sheng Wu, a member of the ETH team.

A possible prototype

This little known and, so far, not particularly useful solid could be the prototype for a new kind of material with potentially technologically interesting properties. For instance, the physicists in Zurich predict that the electric conductivity of such solids should be influenced by magnetic fields in a characteristic way. This phenomenon is also known as magneto-resistance and plays an important role in modern data storage technologies.

Furthermore, the band structure of iridium tetrafluoride has certain peculiarities that have been connected with higher-temperature superconductivity. "All of that's a long shot, of course", Sigrist concedes. Experimental tests of the novel nodal chain metals have still to be done, and surprises are quite possible.

More information: Tomáš Bzdušek et al, Nodal-chain metals, *Nature* (2016). DOI: 10.1038/nature19099

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