Ankylography Permits Three-Dimensional Structure Determination from a Single Sample Orientation

Traditionally, three-dimensional (3D) imaging using coherent diffraction microscopy requires multiple diffraction patterns at different sample orientations. To generate these patterns, precise mechanical tilting or multiple identical copies of a specimen are necessary, thereby preventing 3D imaging by a single x-ray free electron laser (X-FEL) pulse or time-resolved 3D structure determination of disordered materials. J. Miao and K.S. Raines of the University of California, Los Angeles (UCLA), H.C. Kapteyn at the University of Colorado, Boulder, and J. Du at the University of North Texas, and co-researchers, however, have developed a novel imaging technique termed ankylography (from the Greek ankylos for "curved" and graphein for "writing"), which under certain conditions can reconstruct 3D structural information from a single exposure using a monochromatic incident beam. While requiring a similar amount of incident flux to achieve a desired resolution as compared to conventional 3D coherent diffraction microscopy, their approach eliminates the necessity of sample tilting by redistributing the intensities more finely on the Ewald sphere. The researchers state that, with further development, this 3D structure determination method could find broad applications in the physical and life sciences.

As described in the January 14 issue of *Nature* (DOI: 10.1038/nature08705; p. 214), the conceptual design of ankylography begins with a coherent beam illuminating a finite object and the scattered waves forming a diffraction pattern on the Ewald sphere. The researchers demonstrate that when the 2D spherical diffraction pattern is sampled at a sufficiently fine scale, the oversampled diffraction pattern can, in theory, be used to determine the 3D structure of the object. A phase retrieval algorithm that iterates back and forth between Fourier and real space is used to compute the 3D reconstruction. In their studies, the constraints of non-negativity, uniformity outside the support, continuity inside the support, and amplitude extension were applied to facilitate these reconstructions. To confirm the theoretical analysis, 3D numerical reconstructions of a sodium silicate glass structure at 2 Å resolution and a single poliovirus at 2–3 nm resolution were computed using only 2D spherical diffraction patterns. The researchers further demonstrated the experimental feasibility of ankylography by obtaining a 3D image of a test object from a single 2D diffraction pattern taken with a soft x-ray laser.

Because of the oversampling requirement of the single 2D diffraction pattern, in order to compute 3D reconstructions of large specimens at high resolutions, ankylography requires area detectors with a large number of pixels. Additionally, spherical area detectors are more advantageous in reducing interpolation errors. "By incorporating additional constraints into the phase retrieval algorithm and using dedicated detectors," the researchers said that "ankylography could be applied to perform 3D structure determination of a broad range of specimens without the necessity of sample tilting, scanning, or sectioning."

TIFFANY D. ZIEBELL

Electronic Liquid Crystal States Discovered in Parent of Iron-Based Superconductor

An international team of researchers has discovered evidence for electronic liquid crystal states within the parent compound of one type of iron-based, high-temperature (high-T_c) superconductor.

"Because these findings appear similar to what we have observed in the parent state of cuprate superconductors, it suggests this could represent a common factor in the mechanism for high-T_c superconductivity in these two otherwise very different families

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of materials," said team leader Séamus Davis, director of the Center for Emergent Superconductivity at Brookhaven National Laboratory and the J.D. White Distinguished Professor of Physical Sciences at Cornell University. The team of researchers describes their findings, which may help elucidate that long-sought mechanism and lead to higher temperature superconductors, in the January 8 issue of *Science* (DOI: 10.1126/science.1181083; p. 181).

The findings came as a surprise because many theorists had expected the iron-based materials to act more like conventional metal superconductors, where electrons pair up to carry current effortlessly, but without requiring any specific spatial arrangements. These materials must be kept at nearly absolute zero, or -270°C, to operate as superconductors.

In contrast, the newer cuprate and iron-based superconductors operate at a range of warmer, though still chilly, temperatures (e.g., -120°C for cuprates and -220°C for iron-based compounds) that make them potentially more practical for large-scale, real-world applications such as zero-loss power transmission lines. Understanding the mechanism or mechanisms by which they operate could open the door to engineering even warmer, or ideally, room temperature, versions.

The researchers conducted their study through the use of a newly improved and uniquely sensitive spectroscopic image-scanning tunneling microscopy (STM) technique, which allows direct imaging of the arrangements of electrons in materials and exploration of the electronic structure of exquisitely prepared crystals containing calcium, iron, cobalt, and arsenic. A research group at Ames Laboratory led by Paul Canfield, Ames Laboratory Senior Physicist and Iowa State University Distinguished Professor of Physics and Astronomy, fabricated the iron-based crystals.

An important breakthrough was the capability demonstrated by the team to achieve atomically flat and perfectly debris-free surfaces for these studies. Without these conditions the spectroscopic imaging STM techniques cannot be applied. But as soon as the first large-scale images of the electronic arrangements were achieved, it became clear to the team that they were onto something very different than expected.

The researchers observed static, nanoscale arrangements of electrons measuring about eight times the distance between individual iron atoms, all aligned along one crystal axis reminiscent of the way molecules spatially order in a liquid crystal display. They also found that the electrons that are free to travel through the material do so in a direction perpendicular to these aligned electronic liquid crystal states. This demonstrates that the electrons carrying the current are distinct from those apparently aligned in the electronic liquid crystals.

The next step will be to see how these conditions affect the superconductivity of the material when it is transformed to a superconductor.

"Then, if we're able to relate our observations in the iron-based superconductors to what happens in cuprate superconductors, it may help us understand the overall mechanism for high-T_c superconductivity in all of these materials. That understanding could, in turn, help us to engineer new materials with improved superconducting properties for energy applications," Davis said.

In addition to those institutions already mentioned, researchers from the following institutions collaborated on this research: the National High Magnetic Field Laboratory at Florida State University; the University of British Columbia, Vancouver, Canada; and the University of St. Andrews, Scotland.

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