Twisted X-rays unravel the complexity of helical structures

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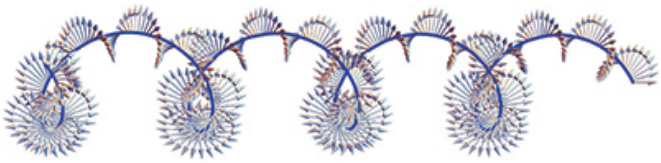

A twisted wave with angular, axial and radial wavenumbers (?, ?, ?) is shown. Credit: Jüstel et al.

Since the discovery of the diffraction of X-rays by crystals just over 100 years ago, X-ray diffraction as a method of structure determination has dominated structural research in materials science and biology. However, many of the most important materials whose structures remain unknown do not readily crystallize as three-dimensional periodic structures. Crystallization can also alter the properties of the material to be studied: a crystallized protein may not function in the way that it would in its natural state, and confining nanostructures such as carbon nanotubes within a crystal lattice can also alter their behaviour.

In the March issue of *Acta Crystallographica Section A*, Jüstel, Friesecke and James propose a new method for studying these kinds of structures, using twisted X-rays [*Acta Cryst.* (2016). A71]. They show that the key to obtaining diffraction data from non-crystalline but symmetric structures, such as helices, lies in matching the symmetry of the incoming radiation to the symmetry of the structure to be studied.

The interesting resonance effects of twisted waves with helical structures suggests that this could be a promising new method for structure determination: send twisted X-rays onto a helical structure, align the waves, the structure and the detector axially, and the outgoing radiation shows sharp, discrete peaks as the incoming wavelength and the amount of twist are varied. Structure prediction from the diffraction pattern then works in exactly the same way as in the case of crystals. Using computer simulations, the authors show that the accuracy of a structure determined using twisted X-rays would be comparable to that obtained by 'classical' X-ray methods.

Remarkably, the method can applied to some of the most important structures in biology and a striking number of the structures that are emerging in nanoscience: buckyballs and many fullerenes, the parts of many viruses, actin, carbon nanotubes (all chiralities), graphene and a large collection of other two-dimensional structures, such as the currently important structures of black phosphorus and the dichalcogenides.

Now someone just has to design the machine to put the twist into the X-rays.

More information: Dominik Jüstel et al. Bragg–von Laue diffraction generalized to twisted X-rays, *Acta Crystallographica Section A Foundations and Advances* (2016). DOI: 10.1107/S2053273315024390

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