FEB 19, 2015

Twisted X-rays: New Methods for The Determination of Noncrystalline Atomic Structure

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ABSTRACT:

A central problem of materials science is to determine atomic structure from macroscopic measurements. Von Laue developed a theoretical method that was put into practice and popularized by Bragg, based on the scattering of plane waves by a crystal lattice. Recently, new structures have emerged like buckyballs (Nobel Prize, Chemistry, 1996) and graphene (Nobel Prize, Physics, 2010), and the third fascinating form of carbon, the carbon nanotube. These have a regular structure but are not crystalline. Regular but noncrystalline structures are also quite common in biology: examples of medical interest include many parts of viruses (such as the 3 helical structures of Ebola), and amyloid protein fibrils that cause diseases like Alzheimer's, Parkinson's and Creutzfeldt-Jakob disease. The discovery of structures like buckyballs, graphene and carbon nanotubes suggests the intriguing possibility that there may well be related, maybe equally interesting but perhaps less common, structures around us, but we cannot "see" them. Thus, the determination of the atomic structure of noncrystalline structures by macroscopic methods is a central problem. After clearing up some fallacies about ordinary x-ray crystallography (Bragg's incorrect picture; the intensity of scattered radiation is not the squared norm of the Fourier transform of the lattice), we propose a new method, which exploits the relationship between structure and the invariance group of Maxwell's equations. We work out the details for helical structures like carbon nanotubes and amyloid protein fibrils. Joint work with Dominik Juestel and Gero Friesecke, TU Munich.

BIOGRAPHY:

Richard James is Distinguished McKnight University Professor in the Department of Aerospace Engineering and Mechanics at the University of Minnesota. He has a Sc.B. in Biomedical Engineering from Brown University and a Ph.D. in Mechanical Engineering from the Johns Hopkins University. He has authored or co-authored some 130 articles, has given 40 plenary and named lectures, and was awarded the Humboldt Senior Research Award (2006/7), the Warner T. Koiter Medal from ASME (2008), the William Prager Medal from the Society of Engineering Science (2008), the Brown Engineering Alumni Medal (2009), and the Theodore von Karman Prize from SIAM (2014, joint with Weinan E). James' research is at the center of mass of mathematics, materials science and mechanics. His current research concerns (i) the study of "Objective Structures", a mathematical way of looking at the structure of matter, (ii) the study of the origins of the reversibility of solid-solid phase transformations, and (iii) the direct conversion of heat to electricity using phase transformations in multiferroic materials.