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Surface / Interface structure / Coherent X-ray diffraction

Crystallography beyond crystals

The basic goal of the crystallographic method is about as fundamental as any in science: the pursuit of structure with an arbitrary level of precision. A broad definition of crystallography merely specifies the method of determination of structure: shining light or particles on an object and collecting for analysis the scattered products. This definition encompasses most of high-energy and nuclear physics, all of microscopy, most of chemistry and biology. The only scientific pursuit left out of this definition is the study of "excitations" of systems, namely reactions, responses, susceptibilities etc. The narrow, but more common, definition of crystallography limits the study to the special case of crystals. My view is that crystallography by the broad definition is alive and healthy, but the specialized interest in crystals alone is dwindling. Given that the name "crystallography" suggests the narrow definition, we might conclude that our field is in decline. Most of the important properties of crystals have already been discovered. Renaming the field to include the broader definition of "structure" is not helpful either because it is not a tangible subdivision of scientific interests.

In my own research experience, I have used traditional (X-ray) crystallographic methods to probe the structure of objects that deviate more and more from the "crystal" paradigm. I have studied the structure of crystal surfaces and interfaces, "defects" such as dislocations and vacancies and most recently the so-called "nanocrystals" that are so small that their physical properties all start to deviate from the classical "bulk". Extrapolating to the future, I seriously expect that we will be able to extend the current crystallographic methodology to crystals as small as a single unit cell, i.e. to non-crystals. An important motivation for this is that the classical crystallographic phase problem can be solved by "oversampling" the diffraction data [1]. This amounts to measuring the diffraction intensity in between the Bragg peaks of a traditional crystal. I am very optimistic about the plans to study the structure of individual biomolecules by spraying them into the beam of a free-electron-laser source of X-rays. The resulting continuous diffraction patterns would be invertible into atomic-resolution images of the molecule. While I believe this is one of the most exciting future directions of our discipline, the method described scarcely qualifies as crystallography by its narrow definition above.

A recent example of my work, which lies along the evolutionary path from macro-crystals to molecules, is shown in the Fig. 1. A micron-sized crystal of gold was studied using a coherent X-ray beam obtained from one of the latest synchrotron radiation sources. The intrinsic coherence of the source was sufficient that interference from the furthest extremities of the nanocrystal is detectable in the diffraction pattern in the form of fringes. Because the diffraction is oversampled, we were able to invert patterns like it to obtain real-space images of the shape of the crystal [2]. I consider this new method to constitute a form of "lensless X-ray microscopy", borrowing the same name that W. L. Bragg gave in 1942 to his method of optical inversion of X-ray diffraction data recorded on photographic film [3].

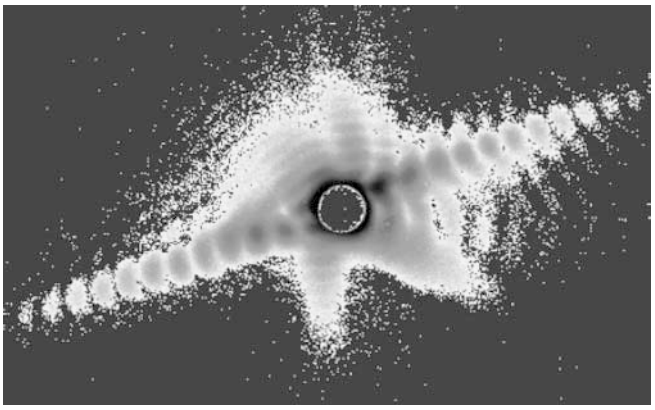

Fig. 1. Shape of the 111 Bragg peak of a micron-sized crystal of gold. This was measured with a coherent, monochromatic beam from the Advanced Photon Source and a CCD detector placed several meters from the sample [2]. A beam stop blocks the intense central region.

As a member of the United States National Committee on Crystallography, I recently attempted to survey the various ways that the subject is taught in the U.S. The results were far from clear because of wide disparities between universities. Crystallography is typically taught separately by several academic departments at the same institution, usually with little correspondence between them. It is most commonly taught as a section of a "methods" or "techniques" course, often occupying just a fraction of a semester in duration. A large number of students are therefore exposed to elementary crystallography, but relatively few learn about the use of space groups. I personally consider that it is the familiarity with space groups that distinguishes a crystallographer from a casual user. One easily spotted trend was the tendency for users of crystallography to unload the responsibility of teaching onto one of the excellent residential "summer schools" run mainly by central laboratories. This last category is the one growth area in crystallographic teaching that was identified in my survey.

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