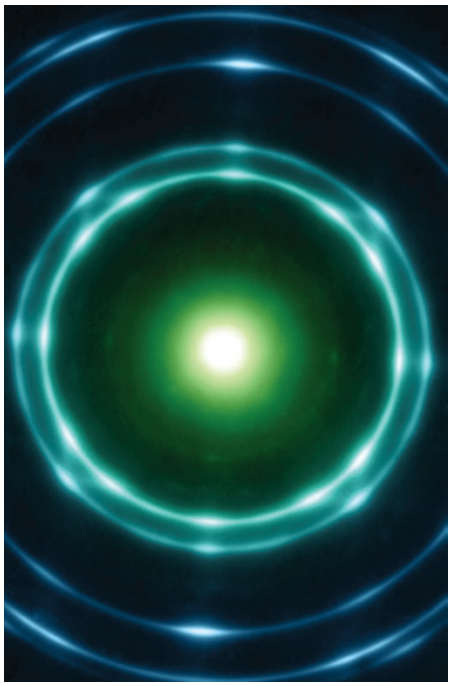
Crystallography matters

Celebrating a field of remarkable depth and importance.

In many ways, crystallography epitomizes the modern scientific era. Max von Laue's pioneering X-ray diffraction experiments in 1912 provided a direct and (with some crucial input from W. Henry and W. Lawrence Bragg) quantifiable link between the macroscopic morphology of crystals and their microscopic atomic structure. The ability to peer inside matter captured the imagination of scientists at the time. This was, after all, a technique that achieved what philosophers had dreamed of for millennia. They weren't to be disappointed: it is fair to say that our understanding of the material world around us — from the constitution of minerals to the molecules that form the basis of life itself — is now rooted in crystallography.

This year marks the centenary of von Laue's Nobel Prize in Physics, which recognized his discovery of X-ray diffraction. This occasion has prompted the General Assembly of the United Nations to designate 2014 as the International Year of Crystallography[1]. With the support of the International Union of Crystallography, which has organized and promoted scientific and cultural events on international, regional and national levels all around the world, the International Year of Crystallography aims to raise awareness and enhance the public profile of the discipline. To complement these activities, *Nature, Nature Materials, Nature Nanotechnology* and *Nature Structural & Molecular Biology* have joined forces to produce a supplement entitled *Nature Milestones in Crystallography*[2], a retrospective that highlights the most significant breakthroughs in the field and underlines its scientific breadth and history.

Most practicing materials scientists will agree that crystallography (and all its related techniques, which include electron microscopy) is ubiquitous in their work. Ironically, however, precisely because it has become such a familiar part of their characterization toolkit, some may take the sheer depth of the insights it provides for granted. A typical example is the widespread notion that crystallography pertains solely to crystals, and that it is somehow merely a tool to probe order in matter. As Philip Ball argues on page 758, diffraction techniques have in fact allowed us to examine a far broader question, namely the extent to which matter can be regarded as ordered. This distinction comes into sharp relief when considering the structure of liquids that, although displaying no long-range order, exhibit a rich variety of short-range spatial and temporal correlations that dictate kinetic and thermodynamic stability constraints that, in the case of water at least, remain incompletely understood[3].



X-ray diffraction of chromium.

Many of the ideas and approaches developed for studying the liquid state also find use in, or even originate from, the study of amorphous systems and powder samples. In their Commentary on page 760, Anthony Cheetham and Andrew Goodwin look back at the main developments in powder crystallography over the past century. Two developments stand out in particular. The first is the iterative approach used to refine the structure of measured samples, now known as the Rietveld method. The second was the realization that the diffuse diffraction rings characteristic of liquids and amorphous phases could be interpreted in terms of pairwise distribution functions (PDFs) that describe the short-range spatial correlations in the structure of these materials. PDFs also give access to temporal correlations between atoms, thus providing a handle on the dynamics of materials responding to external stimuli such as temperature and pressure. In the future, it seems likely that the most profitable use of powder diffraction will, in fact, be in establishing structure–property relationships, rather than in merely determining unknown structures.

Another widespread misconception about crystallography is that it only pertains to the atomic structure of materials. As Steven Bramwell and Bernhard Keimer discuss on page 763, neutron diffraction has provided countless seminal insights that have been crucial to our understanding of the microscopic origin of collective quantum phenomena such as magnetism, superconductivity and superfluidity. Neutrons are themselves magnetic, so they are sensitive to the magnetic moments, or spins, present within a magnetic material. Similarly to the PDF approaches known for disordered materials, neutron diffraction can also be used to measure the correlations between spins. The power of this capability cannot be overstated, and has been at the heart of many of the successful advances witnessed in condensed-matter physics over the past half-century.

Neutron diffraction also offers a reminder that crystallography provides the basis for a unique infrastructure of international laboratories that brings together researchers from across the spectrum of the scientific disciplines. Large-scale scattering facilities, be they neutron or X-ray based, have dramatically increased the collaborative nature of research by providing scientists with high-level resources and expertise, which are often free at the point of use. On page 767, Dimitri Argyriou argues that European neutron science is currently at a crossroads, and careful thought and sustained investment is required to ensure that the European neutron scattering community can continue to thrive.

It is difficult to think of a field that pays as little heed to scientific boundaries as crystallography. Nevertheless, as we hope the Commentaries included in this issue demonstrate, materials science in particular has benefited tremendously from the technique, to the point that it has helped to define our understanding of matter. *Nature Materials* will continue to monitor developments in this discipline closely, and wishes our readers an enjoyable rest of the International Year of Crystallography 2014. ❐

References

1. http://www.iycr2014.org
2. http://www.nature.com/milestones/crystallography
3. *Nature Mater.* **13,** 663 (2014).