



INTRODUCTION

Going from Strength to Strength

IN 1912, THE GERMAN PHYSICIST MAX VON LAUE PUBLISHED THE FIRST PAPER demonstrating x-ray diffraction from a crystal. This discovery, for which he was awarded the Nobel Prize in 1914, provided a window into the regular atomic arrangements within crystals. Today, the Cambridge Structural Database contains more than 600,000 structures of organic and organometallic molecules, many obtained through x-ray crystallography; the Protein Data Bank contains about 100,000 structures. The insights gained from these and other structural studies have revolutionized understanding of chemical and biological systems, leading to the award of 29 Nobel Prizes for scientific achievements related to, or involving the use of, crystallography.

In their Review (p. 1098), Howard and Probert highlight advances in studying single crystals of nonbiological molecules and materials. Novel approaches are helping crystallize unstable samples and mount them in the x-ray diffractometer without damaging the fragile crystals. Advanced x-ray sources allow structures to be obtained from smaller crystals and provide access to time-resolved data on chemical reactions within crystals. Crystals can now be studied at low temperatures and high pressures, further extending the range of conditions and samples that can be structurally characterized.

Garman (p. 1102) charts the history of structural biochemistry, from the initial report of x-ray diffraction from pepsin crystals to the recent characterization of the entire ribosome and of G protein-coupled receptors in different conformational states. She discusses the challenges of protein crystallization, which is increasingly automated. The vast majority of protein structures come from synchrotron beamlines, many of which now offer sample-mounting robots, microfocus beams, and the ability to collect supplementary (e.g., spectroscopic) data. Radiation damage may be overcome through the use of x-ray free-electron lasers. In a related Perspective in *Science Signaling*, Smerdon discusses the insights into the regulation of the kinase mTOR gained from protein crystallography.

Building on the success in obtaining static structures, Miller (p. 1108) discusses efforts to capture atomic motions in crystals in real time. Very bright tabletop electron sources have been used to study photoinduced phase transitions and photoinduced organic reactions. Time-resolved x-ray diffraction experiments are mainly performed at synchrotron light sources, although the development of tabletop instruments is under way. X-ray free-electron lasers offer exciting opportunities for time-resolved studies, particularly of biomolecules.

Science's News writers mark crystallography's centenary with a timeline by Sumner (p. 1092) highlighting some of the field's most celebrated discoveries and advances. Service (p. 1094) describes researchers' long quest for the elusive structures of the proteins that act as gatekeepers to cell membranes. Finally, in News Focus (p. 1072), Service reviews the Protein Structure Initiative, a major research program sponsored by the U.S. National Institutes of Health, and looks ahead to how its scheduled shutdown in 2015 could affect structural biology.

— ROBERT COONTZ, JULIA FAHRENKAMP-UPPENBRINK, MARC LAVINE, VALDA VINSON

Crystallography at 100

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Science

Going from Strength to Strength

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