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Old methods gain new momentum: Laue crystallography

X-ray diffraction is the most powerful method available for the determination of the three-dimensional structure of crystalline materials. Starting from the first Laue diffraction picture recorded in 1912, X-ray crystallography has made remarkable progress and has had profound impact on physics, chemistry, biology and applied sciences such as materials science.

Crystallography as a tool for structural research has had interesting historical developments. Advances in computer technology and high energy physics have invariably led to enhanced power of crystallographic methods. The most remarkable of these developments is the recent application of X-ray diffraction to the study of the dynamical features of biological macromolecules. This has been made possible by the availability of high energy X-ray beams from modern synchrotrons.

Synchrotron radiation differs from conventional X-ray sources such as those from sealed tubes or rotating anode X-ray generators in two important aspects: (a) The intensity of the X-ray beam from a synchrotron source is several orders of magnitude greater than that of the conventional beams, (b) Synchrotron radiation also provides high intensities over a wide wavelength range.

The higher intensity of the synchrotron radiation has been effectively used to study the structures of complex biological macromolecules and their assemblies which crystallize in very large unit cells. The intensities of reflections from these crystals are weak. Also, beams with very low divergence are essential to resolve the crowded X-ray reflections of these crystals. Hence, synchrotron radiation has been instrumental in elucidating the structures of these large biomolecules. It has also been possible to undertake structural studies on radiation sensitive specimens as radiation damage is strongly dependent on the time of exposure and only weakly on the intensity of the beam.

The more dramatic application has been found for the availability of intensities over a wide range of wavelengths. Selecting a particular wavelength for diffraction experiments allows straightforward application of all the earlier techniques but leads to utilization of only a small fraction of the energy available for diffraction experiments. The photographs recorded with the entire available spectrum, the Laue pictures, are much more complex. In these photographs, each reflection not only belongs to a different Bragg plane but also is a result of a different wavelength. The problem of two independent reflections being recorded at the same position on the film, the overlap problem, is also more severe. However, use of the entire spectrum leads to the possibilities of recording the entire diffraction in milliseconds. No reliable method was available for analysing the Laue pictures, despite the fact that they were the first to be recorded. As soon as synchrotron sources became available, ingeneous computer methods were developed for obtaining the intensity spectrum of the radiation source and for estimation of the intensities of individual reflections.

The result of these developments is the ability of determining structures of complex biological macromolecules in millisecond intervals. Hence, it has become possible to follow the structural changes that accompany relatively slow biological processes such as reactions catalysed by certain enzymes. This Laue method has been aptly described as four-dimensional space-time crystallography. The state of the art of this fast developing technique is reviewed in this issue by K. Suguna on page **616**.