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# book reviews

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**Dynamical theory of X-ray diffraction. International Union of Crystallography Monographs on Crystallography** No. 11. Pp. xviii + 661. By André Authier. Oxford: Oxford University Press, 2001. Price GBP 95.00. ISBN 0-19-855960-7.

The story of dynamical diffraction is a curious one. Shortly after Laue's discovery of the diffraction of X-rays, the Braggs measured, and explained in simple concepts, the diffraction of monochromatic X-rays from single crystals. They observed diffraction behavior predicted by dynamical diffraction theory which was fully explained by C. G. Darwin. In fact, Ewald's first theory of dynamical diffraction actually preceded the discovery of X-ray diffraction and, even more remarkably, was an instrument that helped lead to that discovery.

This historical oddity arises from P. P. Ewald's PhD thesis of 1912 and points to a rare event in the history of science. A theory is developed to explain one phenomenon – the double refraction of light. It leads to the question: what would happen if the wavelength of light in the theory is comparable to the spacing of the oscillators? The answer, that the theory made no approximation and was valid for almost any ratio of wavelength to spacing, opened the path towards the discovery of the diffraction of X-rays which, at that time, was one of the most important tools needed to unlock the mystery of the structure of the atom and, subsequently, of all matter that makes up our everyday world.

It is paradoxical that Ewald's theory, which led to the discovery of X-ray diffraction, was hardly needed in the following half century of research to study the physical structure of the crystalline and amorphous materials that fill our earthly world. Instead, the simpler kinematic theory of X-ray diffraction sufficed for most efforts of crystallographers to determine the structure and location of atoms in almost any configuration of scientific and technological interest until the decades of the 1950's and 1960's. Although it had been around for some 30 years, in the early part of the 1950's dynamical diffraction was an esoteric field which one learned about in an advanced course in X-ray diffraction. The theory was used to explain Bragg scattering from natural crystals that were highly perfect. Diamond and calcite are prime examples of such crystals where observed Bragg diffraction curves did not even come close to matching those of most materials whose crystal structure still could be determined using the simple theory for weakly scattering crystals.

However, two developments changed the situation and propelled dynamical diffraction into prominence. First, the transistor was invented and semiconductors grew from minute oddities in the world of crystals to such an important entity that an entire valley in California was named after one of them! Crystals, first of germanium, then of silicon, were grown to become the raw materials of the semiconductor revolution and these, by any measure, were orders of magnitude more perfect than anything nature could produce. X-rays diffracted from them in a manner that could only be understood through the subtleties and complexities of dynamical diffraction, this theory that had interested only a small group of X-ray scientists in the backwaters of crystallographic research in the 20th century.

To understand semiconductor properties, it was necessary to understand the structural details of Ge and Si which demonstrably affected their electrical properties. Understanding every aspect of these crystals was a driving force in solid-state physics and was lavishly funded by the semiconductor industry. These crystals became the platform from which one could launch studies in a wide range of problems in solid-state physics and materials science. For example, studying defects in Ge and Si was easier than in metals because collateral work on purification and crystal growth provided specimens of known progeny, and studying dislocations is much easier in crystals where the defect densities are of the order of $10^3$ cm$^{-2}$ rather than in metals where the density could be many orders of magnitude higher. To study elastic properties and motion of defects in chemically and structurally nearly perfect crystals, X-ray and electron diffraction became the primary tools. For both these techniques, dynamical diffraction was the dominant scattering mode.

The second development was the rise of synchrotron radiation, which turned what had been a waste product of accelerators for high-energy physics into a booming new scientific enterprise. These X-rays had spectacular intensity and brightness and opened new vistas for X-ray research in a manner similar to that in which lasers affected research in physical optics. When the potential for research with this X-radiation was appreciated, machines were developed just to produce synchrotron radiation. The way in which perfect crystals diffracted X-rays was a natural match to the brightness of these new synchrotron beams, and dynamical diffraction from perfect crystals changed from a curiosity of the diffraction of X-rays to the primary means of directing synchrotron radiation to an experimental sample.

Professor Authier has devoted his entire professional career to developing and applying dynamical diffraction theory. In this remarkable book, which is both an in-depth review and a tutorial, he catalogs a half-century of the use of X-rays to study perfect crystals. The book traces the historical development of the field of dynamical diffraction as it has evolved from Ewald's thesis in 1912. Professor Authier divides the work loosely into four parts. The four chapters of Part I give the beginner with a rudimentary knowledge of kinematic diffraction the opportunity to gain facility with the dynamical theory and to acquire a basic understanding of why perfect crystals diffract X-rays in exotic ways. Chapters 1 and 2 give the reader a good physical understanding of dynamical diffraction by presenting the mathematical treatment needed to obtain a working knowledge of how to apply it to real problems and Chapter 4 is an outstanding treatment of many interesting and useful applications of the theory including *Pendellösung*, asymmetric diffraction (an important parameter in high-resolution diffraction and spectroscopy) and the subtleties of the Darwin curves produced when diffracting from the faces of perfect crystals. Chapter 3, present for completeness, is a ten page description of general (ordinary) diffraction theory, but a reader unfamiliar with this would do better to consult one of the standard texts in the field.

Part II has eight chapters on advanced dynamical theory, and deals with the details of intensities and properties of field amplitudes inside the crystal. It points out how Kato's important contributions to spherical-wave treatment justify, for the most part, our use of the simpler but somewhat unrealistic plane-wave approach and points out some cases where the latter treatment fails. In most cases, intensity predictions by the plane-wave theory are virtually the same as in the spherical-wave treatment, but in the particular situation of overlapping wave fields, phase-shift-predicted fringes in certain *Pendellösung* experiments are incorrect. This led to errors in the precise measurement of atomic scattering factors, but Kato's spherical-wave theory correctly explains the results. The more general treatment of the theory by Takagi is presented in Chapter 11. It covers the general case of any incident-wave type, plane or spherical, and is particularly useful for elucidating wave propagation in highly distorted crystals. This section is completed by a chapter on wave tracing and includes the author's seminal work explicitly demonstrating the existence of several branches of the dispersion surface in the two-beam case. In all, this part is an extensive review of the sophistication of the propagation of X-ray Bloch waves in perfect crystals and will be an important resource for the advanced researcher.

Part III has two chapters presenting a detailed treatment of wave propagation in moderately and heavily deformed crystals. It covers many topics, with experimental results from the Paris group (A. Authier, Y. Epelboin, C. Malgrange), and the efforts of U. Bonse, A. Lang, N. Kato, J. R. Patel, D. Taupin and others to study dynamical diffraction effects in these highly deformed crystals and to use the theory to study defects such as stacking faults, growth defects, precipitation, and propagation through and reflection from crystals with externally applied strains.

Part IV has three chapters and covers the coupling of applications of dynamical diffraction to the special properties of synchrotron radiation, providing an important resource for the experimentalist. It addresses crystal optics, topography, standing-wave techniques for atom location, Fresnel zone plates and recent investigations of refractive lenses. Professor Authier covers many of these topics in sufficient depth to give the reader more than a general understanding and he provides up-to-date references that enable one to pursue any of these topics in even greater depth.

Professor Authier has worked on this book over the many years of his dedication to the understanding of the diffraction of X-rays from perfect and nearly perfect crystals. From my point of view, it is a *tour de force*. In 1941, von Laue's book *Roentgenstrahlen Interferenzen* was the seminal treatment for the first 30 years of dynamical diffraction. Professor Authier's book brings us up to the present with a second such treatment of enormous range. He brings us from the nascent period to a description of the field in its most vigorous state. He has given us a historic sense of the evolution of dynamical diffraction, exposed for us its mathematical complexities and shown us how its applications are at the forefront of modern research in solid-state physics and materials science. The book is mandatory reading for specialized workers in dynamical diffraction, and it is an essential reference for anyone interested in modern applications of X-ray scattering using synchrotron radiation.

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**Diffuse neutron scattering from crystalline materials**. By Victoria M. Nield and David A. Keen. Pp. xvi + 317. Oxford: Oxford University Press, 2000. Price GBP 69.50. ISBN 0-19-851790-4.

In this book, the authors have two stated aims. The first is: 'to make diffuse scattering data interpretation more tractable'; the second is: 'to provide an overview of the wide range of available interpretative methods, giving enough information for the reader to select the most useful tool for understanding his or her diffuse data, whilst avoiding elaborate and, to the non-specialist, possibly bemusing detail on any specific methodology'. I believe the authors have been admirably successful in meeting these aims. The book is an accessible and comprehensive guide to diffuse neutron scattering and, though written as an introduction to the technique for graduate scientists, will be a valuable reference text for any crystallographer keen to understand and apply modern interpretative techniques to diffuse scattering data. Though the emphasis of the book is undoubtedly on diffuse *neutron* scattering, with numerous practical examples taken from neutron studies, there is very little material that is not equally of interest to anyone working with X-rays or electrons. The extensive bibliographies at the end of each chapter provide a comprehensive guide to the literature on all aspects of diffuse scattering.

The first chapter gives a brief historical review of the development of interest in diffuse scattering from its earliest beginnings, with the work of such famous names as Debye and Brillouin, to modern times, with current interest extending into protein crystallography. This chapter puts into perspective the special role of neutrons, as opposed to X-rays. The second chapter develops the theory of the basic scattering process specific to neutrons but, even here, X-ray workers will be able to benefit from seeing the differences and similarities in the comparable X-ray scattering theory. The third chapter deals with the theory of diffuse scattering and summarizes the different approaches that have been used to describe it. Important real-space concepts such as short-range-order parameters, size-effect and Huang scattering parameters are described, as well as alternative approaches founded in reciprocal-space descriptions. Again, in this chapter there is very little that is not equally applicable to X-ray scattering. Chapters 4 and 5 deal, respectively, with details of neutron-scattering data collection and data reduction. They provide a succinct description of the different kinds of instruments used and the information that can be obtained from them. Most importantly, reactor and spallation neutron sources are compared, with implications for the types of experiment that can be performed, providing a useful guide for the would-be experimenter. Chapter 6 details how analytical approaches to understanding and analysing diffuse scattering have been progressively replaced by various computer simulation and modelling techniques which allow more complex systems to be studied. Valuable introductions are given to molecular dynamics (MD), Monte Carlo (MC), reverse Monte Carlo (RMC) and the pair distribution function (PDF) methods. The remaining chapters describe, in varying degrees of detail, studies of systems of great diversity. Chapters 7 and 8 deal primarily with the more traditional subjects of substitutional disorder in alloys and simple oxides, and progress to more complex topics, including magnetic systems, quasicrystals and systems that include solvated hydrogen. The special ability of neutrons to see hydrogen and magnetic systems is emphasized. The final chapters concentrate on