

particular interest are the subchapters describing the effects of the size-dependent residence time distribution and the dynamics and control of continuous crystallizers. A short paragraph deals with the plug-flow crystallizer and, again, there is a paragraph on agglomeration. Chapter 9 describes the effect of growth-rate dispersion and methods of analyzing that phenomenon. Chapter 10, on mixing, is very important as, in many cases, mixing has an enormous effect on crystallization. This chapter also includes remarks on fluid-bed crystallizers and series of agitated vessels.

Chapter 11 deals with crystallizer design and operation. It is relatively brief and, besides some general remarks, contains just a few design illustrations using published examples from the literature. The concluding Chapter 12 briefly describes other crystallization techniques, such as adductive and extractive crystallization, the use of hydrotropic additives, and freeze and emulsion crystallization. A few comments are also made on encrustations and modification of crystal habit.

The book contains a number of experimental results and numerous solved examples. In addition, it provides a good literature survey, though in many cases providing only references without detailed descriptions of the respective methods. This is understandable, however, as a more detailed treatment would have enormously expanded the book's size. The book can be recommended as an extremely useful tool for process engineers, technologists and researchers in the field, and to advanced-level students of chemical engineering.

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Atomic and ion collisions in solids and at surfaces.

Edited by ROGER SMITH. Pp. ix + 309. Cambridge: Cambridge University Press, 1997. Price £45.00 (US \$69.95). ISBN 0-521-44022-X.

This book provides a comprehensive survey of various theoretical/computational models available for simulating energetic collisions of atoms with surfaces. Although the book does not address traditional crystallographic methods, it provides the framework for understanding how experimental techniques such as ion scattering spectroscopy (ISS) are sensitive to surface structure. The nine chapters are well organized, and smooth transitions between the various topics demonstrate the editor's skillful coordination of contributions from seven co-authors. While citing many experimental studies along the way, the book focuses on treating the dynamics of atom/surface collisions through non-experimental methods. The text begins with a review of classical scattering theory and the origins of binary collision theory. Throughout, the authors show with clarity and rigor how various standard equations are derived from first principles. It is not assumed that the reader has an advanced degree in physics or mathematics. The authors survey

four basic approaches to modeling dynamics: binary collision theory, transport theory, Monte Carlo techniques, and molecular dynamics simulations. Because an accurate atom/surface potential is required in all computational treatments, a chapter is devoted to the most common semi-empirical methods used for calculating these potentials.

A major theme to the book is understanding the inelastic processes involved when an energetic ion penetrates a lattice. The authors review many models which describe both the excitation of electrons in the solid and the recoil of substrate nuclei brought about by a swift atomic projectile. Discussion focuses on predicting the final rest distribution of the projectiles within the lattice, the corresponding atom displacements induced in the substrate, and sputtering phenomena. Along the way, the authors evaluate many of the popular algorithms and computational packages used in the field, such as *TRIM*, *TRIDYN*, *PRAL*, *KORAL*, *VEGAS*, *MARLOWE* and *SUSPRE*. The authors demonstrate how numerical simulations of ISS, secondary ion mass spectrometry (SIMS), depth profiling, radiation damage, and ion implantation can lead to a greater understanding of the fundamental dynamics. A chapter is also devoted to simulations of the surface topographical changes induced by ion bombardment and deposition. The Editor succeeds in providing a valuable resource for researchers in academia and industry, in fields of surface science, semiconductor engineering, thin-film deposition, and particle-surface interactions, who desire a deeper understanding of the non-experimental ways to study energetic atom/surface collisions. Although the book does not include problems for students, it would make an excellent supporting text for a special topics graduate course. Those interested in structural information will find a description of forward simulations whereby computations accurately reproduce ISS data; however, the inverse problem, *i.e.* extracting a unique surface structure directly from ISS data, has yet to be solved.

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Collected works of Dorothy Crowfoot Hodgkin. Vol.

I. Insulin. Vol. II. Cholesterol, penicillin and other antibiotics. Vol. III. General crystallography and essays. Edited by G. G. DODSON, J. P. GLUSKER, S. RAMASESHAN and K. VENKATESAN. Pp. cxliii + 2230. Bangalore: Indian Academy of Sciences, 1996. Price US \$120 (Individual vols. US \$40). ISBN 81-7296-020-4.

Dorothy Crowfoot Hodgkin was arguably one of the greatest scientists of this century, and certainly one of the most influential figures in the development of crystallography. What motivates such people, and what is it that causes them to inspire

others? Questions like these are the stuff of biographies, yet biographies are necessarily coloured by the people who write them. This collection is far from being a biography. It is in three large volumes, each around 700 pages. It includes all of Dorothy Hodgkin's published works, including scientific papers, essays, reviews and the texts of major lectures. It is supplemented by parts of the autobiographical memoirs that she was working on during the last few years of her life, and is prefaced by a set of personal reminiscences of her life and work, written by some of her co-workers and friends. Yet from this unique combination of materials, Dorothy herself emerges in a subtle and fascinating way. Reading the volumes, I was moved at times, constantly interested, and ultimately left in awe of the person she was and of the enormous pioneering contributions she made to 20th century science.

Even a quick perusal of the table of contents identifies one of the most striking characteristics of her scientific work – her unerring instinct for problems that were of fundamental importance to chemistry, biology and medicine. Here one finds structure analyses of cholesterol, penicillin, vitamin B₁₂ and insulin, all milestones in chemical and biological structure. Added to these are many other studies of steroids, vitamins, antibiotics, proteins and viruses which set the stage for today's explosive growth of research into biological structure, with crystallography at its centre. Materials are not forgotten either, as witnessed by the pioneering 1933 paper written with Bernal on the structures of materials yielding liquid crystals. A glance at her later co-authors also emphasizes her wide influence. They are now spread around the world, often in important positions or with major research groups, forming a vast network of personal and scientific relationships.

The short essays that are placed at the start of each volume provide a unique set of personal reminiscences of Dorothy, of the way she worked, and of the influence she had on others. The contributors include Jack Dunitz, who elegantly identifies her key contributions to chemistry, the particular qualities she brought and the context in which the work was done; Max Perutz, who describes their pioneering studies on proteins and fittingly entitles his essay 'Forty years friendship with Dorothy'; David Phillips, who traces some of the history leading to the establishment of protein crystallography in Oxford; and three from further afield, the late Boris Vainshtein from Russia, S. (Siv) Ramaseshan from India and Dong-Cai Liang and Chih-Chen Wang from China. The latter contributions emphasize her internationalism, for example her role in bringing to the rest of the world the outstanding Chinese research on insulin at a time when that country was a closed book to most Westerners. Siv Ramaseshan, in particular, movingly encapsulates her humanity, her feelings for people, and her influence on science in his country. Many readers in other countries will identify with these sentiments, myself included. Finally, the addresses delivered by Guy Dodson and Max Perutz, at her funeral and at a memorial service in Oxford, complete a beautiful picture of a unique and wonderful person.

It is Dorothy's scientific work that forms the bulk of this collection, however. The first volume comprises all her published work on insulin, together with several special lectures, and her 1965 Nobel Lecture. The second brings together her studies on cholesterol, penicillin, other antibiotics and vitamin B₁₂, and includes personal accounts of the penicillin and B₁₂ work by Barbara Low and Jenny Glusker, respectively. The third is a fascinating mixture of miscellaneous structural analyses, early

studies of protein crystals, book reviews and special lectures, together with her autobiographical memoirs.

There are too many highlights to mention all, but a number of recurring themes emerge throughout the volumes. The first is the way in which she sought to use crystallography as a tool to illuminate chemistry, biology and medicine. Her research began at a time when crystallography was primarily the domain of physics and physicists but, inspired by W. H. Bragg's words that 'by this means you can see atoms in crystals', her pioneering contribution was to apply it to chemistry. Her 1955 *Nature* paper on the crystal structure of the hexacarboxylic acid derived from vitamin B₁₂ is a classic example and her excitement at the significance of the results is obvious: 'To be able to write down a chemical structure very largely from purely crystallographic evidence on the arrangement of atoms in space – and the chemical structure of a quite formidably large molecule at that – is for any crystallographer something of a dream-like situation'. The accounts of the structure analysis of penicillin, whose chemical structure, like that of vitamin B₁₂, was largely unknown prior to the crystallographic work, and which also posed severe crystallographic problems, are also fascinating. And the understated reports on the first diffraction experiments on protein crystals are counterbalanced by Dorothy's own accounts of her excitement at the beautiful patterns and what they promised. The moment in 1935 when she developed the first X-ray photograph of insulin she describes as the most exciting in her life.

A second feature of these writings is her concern with the quality and certainty of results. Many of the conclusions in her original papers are cautious and understated, reflecting her awareness of the need to be right when using a new approach to structure analysis that challenged the traditional chemical methods. The early work on steroids shows the ingenious ways in which trial chemical structures could be tested on crystal packing arguments. Even then, however, she clearly realised that certainty would only come with full X-ray analyses. Modern macromolecular crystallographers, concerned to avoid 'bias' from wrongly introduced atoms, will find the same concerns clearly expressed in the B₁₂ papers from 40 years ago. At the same time, she was determined that the power of crystallography, and the skills of its practitioners, should be given their proper due; Jenny Glusker recounts how Dorothy had a member of her laboratory attend every meeting at which B₁₂ was to be discussed, to make sure of this.

A third source of delight in these writings is to discover how many of the methods used today, especially in macromolecular crystallography, have their precedents in these early structural studies. Isomorphous replacement for phase determination was in the minds of crystallographers from very early on, for example in Bernal's 1935 suggestion that Cd might be substituted for Zn in the newly characterized insulin crystals. It is intriguing to see an *E. coli* mutant used in 1955 to produce a chlorine-substituted vitamin B₁₂ for phase determination and structure confirmation, just as selenomethionine might be used today, and to see that micro-organisms were used to produce a heavy-atom derivative in 1946! Likewise, the structure analysis of another B₁₂ derivative in 1963 provided a beautiful early example of the use of anomalous dispersion as the sole source of phase information. I also note her suggestion, in a 1964 book review, that the experimental evidence for complex structures should be deposited in a central store to allow critical examination – very much a live issue today.

Many other gems are scattered through these pages. Water played an important part in her early protein studies and crystal drying experiments were frequently used to try to learn more about how the protein molecules were organized; much later, this interest is translated into her detailed analysis of the water structure in insulin crystals. Water molecules lie in 'streams' or 'pools', and poorly defined peaks represent 'the stopping places of water molecules moving through the crystal'. There is an account of X-ray diffraction experiments on satellite tobacco necrosis virus crystals in 1944, which began with an accidentally taken still photograph showing their beautiful pattern and ended with an unfortunate accident to the crystal. In the early papers on steroids, there are descriptions of how the optical properties of crystals, their unit-cell dimensions and their diffraction intensity distributions were used with great ingenuity to deduce likely packing arrangements and discriminate between alternative structures.

Dorothy's writing is always direct and frequently testifies to the personal way she thought about molecules and crystals; the structure of vitamin B₁₂ in her 1956 *Nature* paper is introduced by 'The molecule that appears is very beautifully composed ...' and in a discussion of heavy-atom binding to protein crystals she describes molecules that 'casually wander through the crystals, sticking fractionally in a variety of crannies'. There are also comments that should be displayed on the walls of any crystallographic laboratory: one in which she confesses to having 'spent much more of my life not solving structures than solving them' (reassurance for all of us!) and a comment recounted by Barbara Low on the importance of getting all one can from a crystal, no matter how small. 'Crystals are only too small if they have been shown to be. If it is at all possible to do an experiment which might give useful information, do it'.

Other characters also loom large in these volumes. In her Nobel lecture she describes the environment of J. D. Bernal's laboratory in Cambridge in 1932 as one where 'our scientific world ceased to know any boundaries ... we explored the crystallography of a wide variety of natural products, the structure of liquids and particularly water, Rochelle salt, isomorphous replacement and phase determination, metal crystals and pepsin crystals, and speculated about muscle contraction'. Bernal frequently appears as an inspirational figure and there are no fewer than three lectures in which she gives fascinating accounts of his life and works, including descriptions of some

quite extraordinary scientific devices and models. Likewise, there is a wonderful account of the life of Kathleen Lonsdale which equally describes her scientific achievements, including her contributions to the IUCr, and her contributions to prison reform, peace and other social concerns. Other snippets abound: how Max Perutz came to join Bernal as a PhD student; how John Kendrew was drawn into protein crystallography through conversations with Bernal in the jungles of Ceylon; Perutz's account of the successful isomorphous-replacement experiment that gave the breakthrough towards the structure of haemoglobin; and Dorothy's comments on the α -helix and many other milestones in science.

Dorothy's public lectures and essays abound with her humanity and wonderful personal accounts of her scientific life. One I particularly enjoyed is called 'Wandering Scientists', a lecture given in India in honour of Maulana Abul Kalam Azad, which I recommend to every reader for its blend of humanity and science. And to round out the whole picture we have the extraordinary story of her early life, as a child, in Sudan and the Middle East, and the beginnings of her scientific life in Oxford, Cambridge and again in Oxford, as she told it herself in the beginnings of her autobiography.

This collection is a treasure which deserves to be in every library and in every crystallography laboratory. It traces much of the history of crystallography through the life and works of one remarkable person, illuminated by many of the people who knew her and worked with her. It is fascinating to dip into. But readers should be warned ... once you start reading these volumes it is hard to stop and you are likely to find yourself constantly interrupting those around you, to tell them of the latest gem you have read. Professor Ramaseshan, his collaborators, the Raman Research Institute and the Indian Academy of Sciences have done us all a great service in compiling this collection and bringing it to the world in this form.

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