

TOPICAL REVIEW

Direct methods for surface crystallography

D K Saldin and V L Shneerson

Department of Physics, University of Wisconsin-Milwaukee, PO Box 413, Milwaukee, WI 53211, USA

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Online at stacks.iop.org/JPhysCM/20/304208**Abstract**

In the most developed branches of crystallography, structure solution proceeds by two distinct steps: first, an approximate model of the structure is deduced *directly* from the measured data by an algorithm which assumes no preconceived model; second, a process of structure refinement simulates the experimental data for systematic variations of the parameters of such a model and determines a final structure to be that which agrees best with the data. The developments of direct methods for surface crystallography are aimed at enabling the first of these steps to be performed by an objective algorithm applied directly to the experimental data, in order to avoid the (fallible) human guesswork that has been largely applied up to the present to postulate structural models for subsequent refinement.

(Some figures in this article are in colour only in the electronic version)

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1. Introduction

Crystallography is the science of the determination of the atomic-scale structure of repeat units (or *unit cells*) of a crystal from the distribution of the scattering of radiation incident on it. If we restrict our attention initially to the far-field measurement of weak scattering (or single scattering) of an incident plane wave (as is usually the case with x-ray

scattering), the complex amplitudes of the scattered radiation may be regarded as a set of Fourier coefficients of the distribution of scattering matter within each unit cell. If these complex amplitudes may be measured, the recovery of the structure of the unit cell would simply require performing an inverse Fourier transform of those amplitudes. Unfortunately, usual crystallographic experiments measure not these complex amplitudes, but rather their square moduli in the form of diffracted *intensities*. The square roots of these measured intensities are proportional to the (real) amplitudes of the scattered radiation, but the corresponding *phases* are not measured directly.

A major challenge of crystallography is the determination of these phases. In the crystallography of bulk samples, there are two main classes of techniques: those which require information extraneous to the intensities from the diffraction of radiation of a single wavelength, and those which require no further information. In the former class fall three techniques commonly used in protein crystallography, namely multiple isomorphous replacement (MIR) (Green *et al* 1954, Blow and Crick 1959) which requires extra experimental data from related compounds with heavy-atom substitutions; multi-wavelength anomalous dispersion (MAD) (Hendrickson 1991, Leahy *et al* 1992) which requires extra diffraction data from x-rays of wavelengths close to absorption edges of atoms of the sample; and the technique of molecular replacement (Rossman and Blow 1962) which requires a knowledge of the structure

Direct Methods In Crystallography

M. F. C. Ladd, R. A. Palmer



Direct Methods In Crystallography:

Theory and Practice of Direct Methods in Crystallography M. F. C. Ladd, R. A. Palmer, 2012-12-06 Direct methods of crystal structure determination are usually associated with techniques in which phases for a set of structure factors are determined from the corresponding experimental amplitudes by probabilistic calculations. It is thus implied that such ab initio phase calculations do not require a knowledge of atomic positions and this basis distinguishes direct methods from other techniques for structure determination. An acceptably wider interpretation of the term direct methods leads to other important applications involving inter alia the use of heavy atoms, resolution limited phase data for large molecules, rotation functions and Fourier series. These topics are discussed in the later chapters of this book. Although some earlier theoretical investigations were made by Harker and Kaspar, direct methods may be considered to have begun around the year 1950. Important landmarks in the development of the subject include the book by Hauptmann and Karle *The Centrosymmetric Crystal* 1953, the definitive paper by Karle and Karle in *Acta Crystallographica* 1966 and the recent 1978 sophisticated program package MULTAN 78 produced mainly by Germain, Main and Woolfson. Woolfson's book *Direct Methods in Crystallography* was published in 1961 but because of the rapid progress in direct methods much of it soon became outmoded. It is interesting to note that direct methods nearly came into being many years earlier. Certainly the E2 relationship was used implicitly by Lonsdale in 1928 in determining the crystal structure of hexamethylbenzene. *Direct Methods in Crystallography* Carmelo Giacovazzo, 1980. *An Introduction to Direct Methods* Hendrik Schenk, University of Wales (Cardiff), Charles Alfred Taylor, Union internationale de cristallographie. Commission on Crystallographic Teaching, 1984. **Direct Methods, Macromolecular Crystallography And Crystallographic Statistics - Proceedings Of Winter School** H. Schenk, A. J. C. Wilson, S. Parthasarathy, 1987-02-01 Vasopressin is a hormone which has an increasingly important profile. Not only does it play a physiologically significant role in renal water regulation but it also has other renal actions and plays a role in overall cardiovascular control. Even more interesting is the recent growing interest in its potential effects on the brain, notably its influence on specific behaviours. This monograph about the polypeptide vasopressin covers all aspects relating to the production, control of release and actions of this molecule within the body, including its roles as a hormone and as a central neurotransmitter. A consideration of the evolution of the molecule across the species and a brief historical perspective are also included. Clinical conditions associated with hypo and hyper production states are considered together with aspects of treatment in addition to other clinical correlates. **Direct Methods in Crystallography** Michael Mark Woolfson, M. M. Woolfson, 1961. **International Tables for Crystallography, Volume B** Uri Shmueli, 2008-08-27 International Tables for Crystallography are no longer available for purchase from Springer. For further information please contact Wiley Inc, follow the link on the right hand side of this page. Volume B presents accounts of the numerous aspects of reciprocal space in crystallographic research. After an introductory chapter, Part 1 presents the reader

with an account of structure factor formalisms an extensive treatment of the theory algorithms and crystallographic applications of Fourier methods and fundamental as well as advanced treatments of symmetry in reciprocal space In Part 2 these general accounts are followed by detailed expositions of crystallographic statistics the theory of direct methods Patterson techniques isomorphous replacement and anomalous scattering and treatments of the role of electron microscopy and diffraction in crystal structure determination including applications of direct methods to electron crystallography Part 3 deals with applications of reciprocal space to molecular geometry and best plane calculations and contains a treatment of the principles of molecular graphics and modelling and their applications A convergence acceleration method of importance in the computation of approximate lattice sums is presented and the part concludes with a discussion of the Ewald method Part 4 contains treatments of various diffuse scattering phenomena arising from crystal dynamics disorder and low dimensionality liquid crystals and an exposition of the underlying theories and or experimental evidence Polymer crystallography and reciprocal space images of aperiodic crystals are also treated Part 5 of the volume contains introductory treatments of the theory of the interaction of radiation with matter dynamical theory as applied to X ray electron and neutron diffraction techniques The simplified trigonometric expressions for the structure factors in the 230 three dimensional space groups which appeared in Volume I of International Tables for X ray Crystallography are now given in Appendix 1 4 3 to Chapter 1 4 of this volume Volume B is a vital addition to the library of scientists engaged in crystal structure determination crystallographic computing crystal physics and other fields of crystallographic research Graduate students specializing in crystallography will find much material suitable for self study and a rich source of references to the relevant literature

Direct Methods in Crystallography M. M. Woolfson, 1980 Theory and Practice of Direct Methods in Crystallography 3Island Press, 1980-01-31 **Direct Methods in Crystallography** Hubert Phillips, 1961 Direct Methods for Solving Macromolecular Structures S. Fortier, 2013-06-29 This book of the proceedings of the 1997 NATO Advanced Study Institute ASI on Direct Methods for Solving Macromolecular Structures was assembled from the lecturers contributions and represents a comprehensive and in depth overview of crystallographic structure determination methods for macromolecules While having a focus based on the direct methods the Institute adopted an inclusive and broad perspective Thus both direct and experimental phasing techniques are presented in this book highlighting their complementarities and synergies As well methodologies spanning the full crystallographic image reconstruction process from low resolution envelope definition to high resolution atomic refinement are discussed The first part of the book introduces the array of tools currently used in structure determination whether originating from a mathematical computational or experimental framework This section of the book displays the variety and ingenuity of old and new phasing approaches developed to solve increasingly complex structures Some of the contributions focus on recent developments and or implementations that have given older approaches a new life A case in point is the re implementation of Buerger's superposition approach which is now

solving protein structures Another beautiful example is found in the introduction to the traditional multiple isomorphous replacement approach where new techniques such as site directed mutagenesis and the use of inert gases in the preparation of heavy atom derivatives are described Equally impressive are the presentations of newer approaches which take advantage of advances on the experimental front e g **Direct Methods of Solving Crystal Structures** Henk Schenk,1991 Proceedings of the 18th course of the International School of Crystallography held April 1990 in Erice Italy Annotation copyrighted by Book News Inc Portland OR [Direct Methods in Crystallography, By M.M. Woolfson](#) Michael Mark Woolfson,1963 **Introduction to Macromolecular Crystallography** Alexander McPherson,2011-09-20 A comprehensive and approachable introduction to crystallography now updated in a valuable new edition The Second Edition of this well received book continues to offer the most concise authoritative and easy to follow introduction to the field of crystallography Dedicated to providing a complete basic presentation of the subject that does not assume a background in physics or math the book s content flows logically from basic principles to methods such as those for solving phase problems interpretation of Patterson maps and the difference Fourier method the fundamental theory of diffraction and the properties of crystals and applications in determining macromolecular structure This new edition includes a vast amount of carefully updated materials as well as two completely new chapters on recording and compiling X ray data and growing crystals of proteins and other macromolecules Richly illustrated throughout to clarify difficult concepts this book takes a non technical approach to crystallography that is ideal for professionals and graduate students in structural biology biophysics biochemistry and molecular biology who are studying the subject for the first time **Physical and Direct Methods in Crystallography** Adam Charles Ralph,1991 **International Tables for Crystallography, Volume B** U. Shmueli,2008-08-25 International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science Volume B presents accounts of the numerous aspects of reciprocal space in crystallographic research This volume is a vital addition to the library of scientists engaged in crystal structure determination crystallographic computing crystal physics and other fields of crystallographic research Graduate students specializing in crystallography will find much material suitable for self study and a rich source of references to the relevant literature New to this edition A new chapter on modern extensions of the Ewald method for Coulomb interactions in crystals Three new sections on electron diffraction and electron microscopy in structure determination describing point group and space group determination by convergent beam electron diffraction three dimensional reconstruction and single particle reconstruction Substantial revisions to the chapters on space group representations in reciprocal space direct methods Patterson and molecular replacement techniques and disorder diffuse scattering More information on the series can be found at <http://it.iucr.org> **Direct Methods in Crystallography** ,1980 **Direct Methods in Crystallography** International Union of Crystallography,Medical Foundation of Buffalo (N.Y.). Research Laboratories,1976 **International Tables for Crystallography, Volume F** Eddy Arnold,Daniel M.

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d local tournaments hosted by jka dojos 2 all tournaments in all countries shall abide by this present document item 3 rules of conduct for all participants all participants shall act in accordance to the highest standards of ability and of fair play in the spirit of karate do and strive to the utmost respect and dignity towards

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rules regulations for the 2019 jing an international elite challenge asia pacific kyokushin karate elite invitational tournament and the 1st 国家 全国 锦标赛 i mission statement of the tournament promotion of karate as a sport and enhancement of karate training in china ii sponsoring organizations lead sponsor

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q what tournament rules apply in kwf tournaments a kyokushin world federation will use the standard kyokushin karate rules introduced to us by sosai oyama tournaments shall include full contact kumite competition both for men and women as well as kata competition

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november 17 and 18 2023 in arnhem the netherlands will be held kwf world kyokushin karate championships among children juniors and seniors thursday november 16 12 00 19 00 registration of the teams 20 00 22 00 referee briefing t b d general meeting friday november 17 6 tatami 10 00 12 00 kata championships all categories

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karate styles embracing these rules are often called knockdown karate styles and these include both organizations that originated from kyokushin such as shidōkan karate ashihara karate enshin karate shindenkai and seidokaikan the style that originated the k 1 as well as styles that originated independently from kyokushin such as

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each opponent faced will be fresh and not fatigued or injured each of the rounds are done under test conditions where either of the fighters are allowed to deliver knock out blows the challenge was devised by masutatsu oyama the founder of kyokushin and

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normally knockdown rules include no protectors or guards are used with exception to groin guards and teeth protection 3 minutes match time the fighter that achieves an ippon one point will win the match and the fight is stopped

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5 fight duration the length of each round is one minute match times may be extended up to 2 minutes if divisions are under 5 opponents 6 legal techniques no head contact open hand strikes punches elbow strikes knee kicks and straight kicks to the body and legs circular kicks to the body and legs

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rules all world open tournaments operate under knockdown karate rules which involve standup bareknuckle fighting with basically no protection the more characteristic rules in knockdown karate compared to other styles are that you are not allowed to punch in the face and a point system that only counts hits that actually hurt the opponent

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kyokushin is the basis of glove karate a knockdown karate format wearing boxing gloves and allowing punches to the head glove karate rules are used in kyokushin karate iran in popular culture kyokushin karate has featured in following videogames the move sets of ryu and ken from capcom's street fighter franchise are based on kyokushin

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oct 21 2023 adult rules apply for those 15 and up oshi sweeping sabaki above elbow etc the divisions will be determined by the entries received every effort will be made to match fighters on weight grade age experience etc depending on the number of entries received matches may take the form of

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