

and hexagonal lattices. Furthermore, the point group $\bar{3}m$ in the hexagonal description is further subdivided into two cases – one having the normal of the mirror planes in the [100] direction and the other one having the normal in the [210] direction. The Laue group $2/m$ is also subdivided into two cases – with the b axis unique and with the c axis unique.

Since the distribution of the X-ray intensity $I(hkl)$ in reciprocal space shows the same symmetry as a general crystal form of the corresponding Laue class, the asymmetric unit of X-ray intensity data for a crystal is the same as that for the crystal forms $\{hkl\}$ with the symmetry of its Laue group.

Table 1 shows information on the 11 Laue groups (column 3). The crystal system is given in column 1, all corresponding noncentrosymmetric point groups are listed

in column 2. Column 4 describes one asymmetric unit for the intensity data of each Laue group. Alternative possibilities are separated by dashed lines. The last column shows the fraction of reciprocal space belonging to one asymmetric unit.

This work was supported by the Korean Science and Engineering Foundation (KOSEF) through the Science Research Center (SRC) of Excellence Program.

References

- SAKURAI, T. (1986). *A Practical Guide for X-ray Crystal Structure Analysis*, p. 54. Tokyo: Syokabo.
 STOUT, G. H. & JENSEN, L. H. (1989). *X-ray Structure Determination*, pp. 159–162. New York: Wiley.

International Union of Crystallography

Acta Cryst. (1993). **A49**, 371–373

International Tables for Crystallography

**Volume C: Mathematical,
Physical and Chemical Tables**
Editor: A. J. C. Wilson

Volume C is the result of many years of collaborative effort to revise and update Volumes II, III and IV of *International Tables for X-ray Crystallography*. Most of the contributions are entirely new; the remaining sections are the result of editorial condensation of material from the earlier volumes or have been revised by their original authors. Copies may be ordered directly from the publishers (Kluwer Academic Publishers, PO Box 17, 3300 AA Dordrecht, The Netherlands), from Polycrystal Book Service, Box 3439, Dayton, Ohio 45401, USA, or from any bookseller. [Price Dfl 400 (or Dfl 200 for individuals, who should give a written undertaking that the copy is for their personal use only and will not be made available to libraries *etc.*.)]

A full review will be published in *Acta Crystallographica*, Section A.

Table of Contents

PREFACE

PART 1: CRYSTAL GEOMETRY AND SYMMETRY

- 1.1. Summary of general formulae (E. Koch)
- 1.2. Application to the crystal systems (E. Koch)
- 1.3. Twinning (E. Koch)
- 1.4. Arithmetic crystal classes (A. J. C. Wilson)

PART 2: DIFFRACTION GEOMETRY AND ITS PRACTICAL REALIZATION

- 2.1. Classification of experimental techniques (J. R. Helliwell)
- 2.2. Single-crystal X-ray techniques (J. R. Helliwell)
- 2.3. Powder and related techniques: X-ray techniques (W. Parrish)
- 2.4. Powder and related techniques: electron and neutron techniques
 - 2.4.1. Electron techniques (J. M. Cowley)
 - 2.4.2. Neutron techniques (A. W. Hewat)
- 2.5. Energy-dispersive techniques
 - 2.5.1. Techniques for X-rays (B. Buras and L. Gerward)
 - 2.5.2. White-beam and time-of-flight neutron diffraction (J. D. Jorgensen, W. I. F. David and B. T. M. Willis)
- 2.6. Small-angle techniques
 - 2.6.1. X-ray techniques (O. Glatter)
 - 2.6.2. Neutron techniques (R. May)
- 2.7. Topography (A. R. Lang)

PART 3: PREPARATION AND EXAMINATION OF SPECIMENS

- 3.1. Investigation and selection of crystals (C. H. MacGillavry and N. F. M. Henry)
- 3.2. Determination of the density of solids (F. M. Richards)
- 3.3. Measurement of refractive index (E. S. Larsen Jr and R. Meyrowitz)
- 3.4. Mounting and setting of specimens for X-ray crystallographic studies (P. F. Lindley)
- 3.5. Preparation of specimens for electron diffraction and electron microscopy (N. J. Tighe, J. R. Fryer and H. M. Flower)
- 3.6. Specimens for neutron diffraction (B. T. M. Willis)

PART 4: PRODUCTION AND PROPERTIES OF RADIATIONS

- 4.1. **Radiations used in crystallography** (V. Valvoda)
- 4.2. **X-rays**
- 4.2.1. Generation of X-rays (U. W. Arndt)
- 4.2.2. X-ray wavelengths (U. W. Arndt)
- 4.2.3. X-ray absorption spectra (D. C. Creagh)
- 4.2.4. X-ray absorption (or attenuation) coefficients (D. C. Creagh and J. H. Hubbell)
- 4.2.5. Filters and monochromators (A. J. C. Wilson)
- 4.2.6. X-ray dispersion corrections (D. C. Creagh and W. J. McAuley)
- 4.3. **Electron diffraction**
- 4.3.1. Scattering factors for the diffraction of electrons by crystalline solids (J. M. Cowley)
- 4.3.2. Relativistic parameters as a function of accelerating voltage
- 4.3.3. Complex scattering factors for the diffraction of electrons by gases (A. W. Ross, M. Fink and R. Hilderbrandt)
- 4.3.4. Electron energy-loss spectroscopy on solids (C. Colliex)
- 4.3.5. Oriented texture patterns (B. B. Zvyagin)
- 4.3.6. Computation of dynamical wave amplitudes
- 4.3.6.1. The multislice method (D. F. Lynch)
- 4.3.6.2. The Bloch wave method (A. Howie)
- 4.3.7. Measurement of structure factors and determination of crystal thickness by electron diffraction (J. Gjønnes and J. W. Steeds)
- 4.3.8. Crystal structure determination by high-resolution electron microscopy (J. C. H. Spence and J. M. Cowley)
- 4.4. **Neutron techniques**
- 4.4.1. Production of neutrons (G. Lander)
- 4.4.2. Devices for neutron beam definition (A. K. Freund and G. Dolling)
- 4.4.3. Resolution functions (R. Pynn and J. M. Rowe)
- 4.4.4. Scattering lengths for neutrons (V. F. Sears)
- 4.4.5. Magnetic form factors (P. J. Brown)
- 4.4.6. Absorption coefficients for neutrons (B. T. M. Willis)

PART 5: DETERMINATION OF LATTICE PARAMETERS

- 5.1. **Introduction** (A. J. C. Wilson)
- 5.2. **X-ray diffraction methods: polycrystalline** (W. Parrish and A. J. C. Wilson)
- 5.3. **X-ray diffraction methods: single crystal** (E. Galdecka)
- 5.4. **Electron-diffraction methods**
- 5.4.1. Determination of cell parameters from single-crystal patterns (A. W. S. Johnson)
- 5.4.2. Kikuchi and HOLZ techniques (A. Olsen)
- 5.5. **Neutron methods** (B. T. M. Willis)

PART 6: INTERPRETATION OF DIFFRACTED INTENSITIES

- 6.1. **Intensity of diffracted intensities**
- 6.1.1. X-ray scattering (E. N. Maslen, A. G. Fox and M. A. O'Keefe)
- 6.1.2. Magnetic scattering of neutrons (P. J. Brown)
- 6.1.3. Nuclear scattering of neutrons (B. T. M. Willis)
- 6.2. **Trigonometric intensity factors** (H. Lipson)
- 6.3. **X-ray absorption** (E. N. Maslen)
- 6.4. **The flow of radiation in a real crystal** (T. M. Sabine)

PART 7: MEASUREMENT OF INTENSITIES

- 7.1. **Detectors for X-rays**
- 7.1.1. Photographic film (P. M. de Wolff)
- 7.1.2. Geiger counters (W. Parrish)
- 7.1.3. Proportional counters (W. Parrish)
- 7.1.4. Scintillation and solid-state detectors (W. Parrish)
- 7.1.5. Energy-dispersive detectors (B. Buras and L. Gerward)
- 7.1.6. Position-sensitive detectors (U. W. Arndt)
- 7.1.7. X-ray-sensitive TV cameras (J. Chikawa)
- 7.1.8. Storage phosphors (Y. Amemiya and J. Chikawa)
- 7.2. **Detectors for electrons** (J. N. Chapman)
- 7.3. **Thermal neutron detection** (P. Convert and P. Chieux)
- 7.4. **Correction of systematic errors**
- 7.4.1. Absorption
- 7.4.2. Thermal diffuse scattering (B. T. M. Willis)
- 7.4.3. Compton scattering (N. G. Alexandropoulos and M. J. Cooper)
- 7.4.4. White radiation and other sources of background (P. Suortti)
- 7.5. **Statistical fluctuations** (A. J. C. Wilson)

PART 8: REFINEMENT OF STRUCTURAL PARAMETERS

- 8.1. **Least squares** (E. Prince and P. T. Boggs)
- 8.2. **Other refinement methods** (E. Prince and D. M. Collins)
- 8.3. **Constraints and restraints in refinement** (E. Prince, L. W. Finger and J. H. Konnert)
- 8.4. **Statistical significance tests** (E. Prince and C. H. Spiegelman)
- 8.5. **Detection and treatment of systematic error** (E. Prince and C. H. Spiegelman)
- 8.6. **The Rietveld method** (B. T. M. Willis and A. Albinati)
- 8.7. **Analysis of charge and spin densities** (P. Coppens and P. J. Becker)
- 8.8. **Accurate structure-factor determination with electron diffraction** (J. Gjønnes)

PART 9: BASIC STRUCTURAL FEATURES

9.1. Sphere packings and packings of ellipsoids

(E. Koch and W. Fischer)

9.2. Layer stacking

9.2.1. Layer stacking in close-packed structures
(D. Pandey and P. Krishna)9.2.2. Layer stacking in general polytypic structures
(S. Durovič)

9.3. Typical interatomic distances: metals

(L. D. Calvert)

9.4. Typical interatomic distances: inorganic compounds

(G. Bergerhoff)

9.5. Typical interatomic distances: organic compounds

(F. H. Allen, O. Kennard, D. G. Watson,
L. Brammer, A. G. Orpen and R. Taylor)

9.6. Typical interatomic distances: organometallic compounds and coordination complexes of the

d- and *f*-block metals (A. G. Orpen, L. Brammer,
F. H. Allen, O. Kennard, D. G. Watson and
R. Taylor)

9.7. The space-group distribution of molecular organic structures

(A. J. C. Wilson)

9.8. Incommensurate and commensurate modulated structures

(T. Janssen, A. Janner, A. Looijenga-Vos
and P. M. de Wolff)

PART 10: PRECAUTIONS AGAINST RADIATION INJURY

(D. C. Creagh and S. Martinez-Carrera)

AUTHOR INDEX

SUBJECT INDEX

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, USA). As far as practicable, books will be reviewed in a country different from that of publication.

Acta Cryst. (1993). **A49**, 373–374

Fundamentals of crystallography. By C. GIACOVAZZO, H. L. MONACO, D. VITERBO, F. SCORDARI, G. GILLI, G. ZANOTTI and M. CATTI. (*IUCr Texts on Crystallography* No. 2.) Pp. xv + 654. Oxford: International Union of Crystallography/Oxford University Press, 1992. Price £27.50 (paperback), £62.00 (hardback). ISBN 0-19-855578-4 (p/b), 0-19-85579-2 (h/b).

For this book, the second of the new IUCr Texts on Crystallography, Carmelo Giacovazzo has edited, revised, expanded and brought up to date in English translation *Introduzione alla Cristallografia Moderna*, first published in 1985. The stated aim of the book is to provide a compact comprehensive account of modern crystallographic subjects that should be useful as a text for university courses that cover crystallography, fully or only partially, but that should also be of use at the doctoral or research level. I believe that this book more than adequately meets these goals and the high quality of the translation should ensure it a significantly wider audience than that reached by the original.

Recognizing the interdisciplinary character of modern crystallography, the editor realized that a book of this kind would need to be written by several authors and that the various contributions would have to be 'carefully harmonized in order to conform them to a unified plan'. The result is a text that can be used with profit in its entirety but from which instructors and students can select according to their particular interests. There are three core chapters. Chapter 1 (Giacovazzo, 60 pp.) is a concise treatment of symmetry in crystals. The first half covers symmetry elements, lattices, point groups, Laue classes, crystal systems, Bravais lattices, and plane, line and space groups. This material is fundamental for audiences at all levels.

For the more advanced student, the second half of the chapter consists of appendices dealing with isometric transformations, combinations of movements, Wigner–Seitz cells, space-group rotation matrices, symmetry groups and generalized symmetry with an introduction to *G* groups and color symmetry. Very usefully, in this last case, actual structural arrangements are used as illustrations. The second core chapter (Chapter 3, Giacovazzo, 86 pp.) covers the diffraction of X-rays by crystals. The same division between fundamental and more advanced topics is adopted here. The treatment is kinematic, with a progression from scattering by electrons to that by atoms, molecules and crystals. There are good treatments of symmetry in reciprocal space and of anomalous dispersion, and a short introduction to modulated structures. The appendices here deal with the mathematics of Fourier transforms and convolution operations, and with more subtle aspects of scattering such as Compton scattering, the anisotropic temperature factor, the Renninger effect and electron and neutron scattering. Scattering by non-crystalline materials such as gases, liquids and amorphous solids is covered, as is small-angle scattering. Two final appendices deal with electron-density mapping and a more advanced look at modulated structures and quasicrystals.

For the newcomer to crystallography, the third core chapter (Chapter 5, Viterbo, 79 pp.) deals with the solution and refinement of crystal structures. After a general introduction come sections dealing with the statistical analysis of structure amplitudes, the use of the Patterson method and direct methods, and refinement by least-squares and difference Fourier methods, with a short discussion of the determination of absolute configuration. For the more experienced reader, the appendices deal with structure-factor and triplet-invariant probability distributions, Patterson vector methods, pseudotranslational symmetry, magic integers and newer multisolution methods and procedures for completing a partial model. As is the case for the other core chapters, the references here are particularly helpful and cover the literature into 1990.