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Fundamentals of Crystallography, 3rd edition. By C. Giacovazzo, H. L. Monaco, G. Artioli, D. Viterbo, M. Milaneso, G. Ferraris, G. Gilli, P. Gilli, G. Zanotti and M. Catti. Edited by C. Giacovazzo. IUCr Texts on Crystallography No. 15, IUCr/Oxford University Press, 2011. Pp. xxi + 842. Price (hardback) GBP 90.00. ISBN 978-0-19-957365-3.

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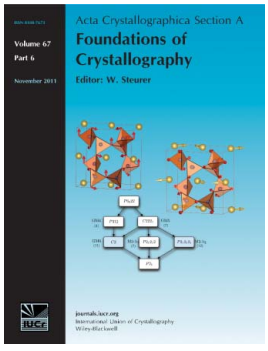

Acta Crystallographica Section A: Foundations of Crystallography covers theoretical and fundamental aspects of the structure of matter. The journal is the prime forum for research in diffraction physics and the theory of crystallographic structure determination by diffraction methods using X-rays, neutrons and electrons. The structures include periodic and aperiodic crystals, and non-periodic disordered materials, and the corresponding Bragg, satellite and diffuse scattering, thermal motion and symmetry aspects. Spatial resolutions range from the subatomic domain in charge-density studies to nanodimensional imperfections such as dislocations and twin walls. The chemistry encompasses metals, alloys, and inorganic, organic and biological materials. Structure prediction and properties such as the theory of phase transformations are also covered.

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book reviews

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Fundamentals of Crystallography, 3rd edition. By C. Giacovazzo, H. L. Monaco, G. Artioli, D. Viterbo, M. Milaneso, G. Ferraris, G. Gilli, P. Gilli, G. Zanotti and M. Catti. Edited by C. Giacovazzo. IUCr Texts on Crystallography No. 15, IUCr/Oxford University Press, 2011. Pp. xxi + 842. Price (hardback) GBP 90.00. ISBN 978-0-19-957365-3.

Fundamentals of Crystallography is a reference textbook which gets updated every ten years, the previous editions dating back to 1992 and 2002, respectively (a 'zeroth' edition was published in Italian under the title *Introduzione alla Cristallografia Moderna* in 1985). Reviews of the previous editions were published in *Acta Cryst.* (1993). A**49**, 373–374 and *Acta Cryst.* (2003). A**59**, 200. One reason why it is worth analysing in some detail the content of this book, rather than just pointing out the changes with respect to the previous edition, is the brevity of these reviews.

The area covered is so vast and wide that to perform a complete in-depth review of all the chapters would need a co-operative work by specialists of many different fields, as is the case for the authors of this collective textbook. This review is inevitably slightly biased by the reviewer's background and competences, or rather lack of, but it will hopefully be of some help for future improvements.

A number of updates have been introduced in this new edition, which span from new figures (in practically all the chapters) to rewritten sections (like those on powder crystallography and electron diffraction) to entirely new sections (humidity control of macromolecular crystals). This big effort to reflect the state of the art and provide up-to-date knowledge is particularly welcome in a textbook that is presented as one of the main references in the field (note, however, that the term 'recent', often used with reference to articles that were such when previous editions of the book were published, should have been updated too). Unfortunately, some errors and imperfections that affected the previous editions are still present, while some topics that should have finally found their place are still absent.

The ten chapters of the book could ideally be divided into four sections: fundamentals (Chapters 1–4), experimental methods and techniques (Chapters 5–6), structures (Chapters 7–9), and physical properties (Chapter 10). Crystal optics is reduced to two pages in Chapter 10, and this reflects the unfortunate fate of what used to be part of the fundamental background of a crystallographer. For a book published in the series *IUCr Texts on Crystallography*, one would expect a more rigorous terminology and a stricter adhesion to the standards settled in *International Tables for Crystallography* (hereafter indicated as *IT*, and in particular *ITA* for Volume A). Unfortunately, a sort of laboratory jargon is widely used in several chapters, which complicates the transition to *IT*: this is the original sin of a book that should be a clear guide and introduction to the less easily digestible text parts of *ITA*.

Chapter 1 introduces symmetry in direct space. It counts 38 pages where fundamental concepts are introduced, plus 26 pages of appendices where some matrix algebra and the definition of a symmetry group are introduced. The choice of putting the latter in an appendix is hardly understandable, but this is far from being the only problem in the chapter.

Despite the absolutely general target and purpose of the title, the reader learns that a crystal is 'made of molecules or group of molecules,' a definition which would automatically exclude the bulk of (truly) inorganic crystals. However, a few lines before we read about 'macromolecules of silicon dioxide' in glass and we understand that this wording is simply jargon which, unluckily, is widely diffused today: the day when we read about the 'NaCl molecule' the dark side of crystallography will have got its revenge.

Another rather disturbing use of terms outside their meaning is the confusion among 'element', 'operation' and 'operator', which we also find in the following chapters. Apart from the fact that *ITA*, with very few exceptions, avoids the term 'operator', the use of 'operation' (the transformation) instead of 'element' (the geometric element about which this operation is performed) and *vice versa* is surprising in a text like this. Also, the systematic use of lattice point instead of lattice node goes against the standards.

A conceptual weakness shows up when lattices and crystal systems are introduced: the criterion for defining a crystal system ('unit cells of the same type') is actually the one that defines the crystal family (never mentioned in the book) through its conventional cell (seldom used in the book, but never defined). As a consequence, the trigonal and hexagonal systems are introduced together: indeed, they belong to the same crystal family, while for crystal systems the minimal common set of macroscopic symmetry operations has to be considered. (For a more general, rigorous and abstract definition, see Part 8 in *ITA*.)

The Bravais lattices are then introduced on the basis of the conventional cell (which has not been defined: see instead Section 2.1.3 in *ITA*) and a 'trigonal lattice' shows up instead of the rhombohedral lattice. This seems to be a common problem in Latin countries: Italians always use trigonal, French always use rhombohedral and it seems very hard to convince either of them that the two words are not synonymous (trigonal is a crystal system, rhombohedral is a type of lattice, as well as a lattice system). Without this confusion, one would have expected to find it clearly stated that for rhombohedral space groups only two symbols after the lattice type occur in the Hermann–Mauguin symbol, because in a

rhombohedral space group there are only two independent symmetry directions, whereas three symbols are given for 'hexagonal and trigonal groups' (p. 28).

At p. 29 we read that 'in short symbols symmetry planes are suppressed as much as possible,' while what is suppressed are the axes. A few lines below we find that 'Symmetry elements at h also occur at $h + \frac{1}{2}$,' whereas this applies only to twofold elements.

A few more imperfections. The brick wall on the right part of Fig. 1.7 is not periodic but in twin orientation, the primitive cells on the right being rotated 90° clockwise with respect to those on the left (the upper part of the figure is again different); simplification of Miller indices for planes parallel to a face should have been applied (p. 9); the orthohexagonal cell is called 'a centred rectangular cell', while the H and D cells are not mentioned; in the list of symmetry elements the glide plane e is missing, even though it has the second highest priority in *ITA* in defining the space-group symbol; on p. 30 a comparison is made between $P2_12_12_1$ and ... $P2_12_12_1$ (probably a typographical error for $P2_12_12$); set of equivalent directions should be indicated in angular, not square, brackets; in the definition of proper subgroup (Appendix 1.E.1) the exclusion of {1} is missing; the standard name for the G_1^2 groups is frieze groups, not border groups; the number of G_4^4 groups is 4894, not 4895 (p. 62); space-group symbols should have the capital letters, indicating the type of lattice, in italics.

Chapter 2 deals with crystallographic computing. In this chapter (75 pages plus 10 pages of appendices) we find the metric tensor, the reciprocal lattice, basis transformations, examples of crystallographic calculations, definitions of the Niggli cells, derivative lattices, coincidence-site lattices, directions for how to compute electron density and structure factors (defined only in Chapter 3), a long presentation of the least-squares method, followed by a shorter introduction to alternative methods (maximum likelihood and gradient methods), followed by a section on powder crystallography (peak search, Rietveld refinement), the effect of thermal motion and the accuracy of calculated parameters. The appendices present examples of transformations and calculations.

The choice of describing refinement strategies and algorithms before diffraction and the phase problem clearly shows that the book is not addressed to a beginner but rather to a user who already has a clear idea of crystallographic practice and needs to gain in-depth understanding. Furthermore, the divergence from the IUCr standards and a certain lack of rigorousness in the language is disturbing. In *ITA*, covariant and contravariant components are written as row matrices and column matrices, respectively. In this chapter, column matrices are systematically used, which obliges one to use the inverse-transpose matrix, instead of the inverse, when applying a transformation of the basis to the coordinates or *vice versa*. The terms 'sublattice' and 'superlattice' are used with opposite meaning with respect to *ITA*. A sublattice corresponds to a subgroup of translations: the *ITA* use is definitely better and should have been followed. The 'some non-centrosymmetric space groups' for which 'the origin may float in some directions' are the pyroelectric groups, which should have been defined before. The local symmetry is here erroneously called 'non-crystallographic symmetry' (p. 114); unfortunately, this mistake is quite common in the literature. [For a discussion about this problem, see *Z. Kristallogr.* (2008). **223**, 605–606.] In Appendix 2B the fact that the angle between two reciprocal-lattice vectors is always called the 'angle between two planes,' for historical reasons, while it is actually the supplement of it, should have been mentioned. The reciprocal-lattice planes should have been indicated with an asterisk (*).

Chapter 3 deals with X-ray diffraction by crystals (76 pages of which 40 are appendices). In fact, despite the title, neutron and electron diffraction are also discussed (in the appendices: this explains their length), although more briefly, and a comparison among the three approaches is addressed. Both the physics and the mathematics of the topic are presented clearly and with the necessary depth, but here again deviations from standards occur, like at p. 192: the 'centring order of the cell' should have been called multiplicity and the 'multiplicity factor of the Laue class' is actually the order. One may remark that Röntgen's paper was published in 1895 (28 December), not 1896 as stated on p. 157.

Chapter 4 goes 'beyond ideal crystals' in 43 pages, of which 13 are appendices, presenting a series of cases which increasingly diverge from the simple crystalline state: twins, modulated structures, quasi-crystals, mesomorphic phases ('liquid crystals'), paracrystals, amorphous and liquids, up to gases, as well as the scattering produced by them and a brief account of the corresponding mathematical treatment. This chapter alone could have taken the whole length of the book; it is here presented at a reasonably introductory level which, nevertheless, gives the reader a clear idea of the complexity as well as how the different subjects are approached. The section on twins should have been updated to reflect results obtained since the previous editions, and to correct some imprecise statements and expressions. The sentence 'TLS twins are optically indistinguishable' is misleading: here it is meant that the geometry of the diffraction pattern is not a clue for twin detection because there is no splitting of reflections. 'Optically indistinguishable' means that they cannot be distinguished by observation in the optical microscope, which is not true for twinning by reticular merohedry, where the extinction of polarized light does not occur simultaneously for the twinned individuals. The improper term 'merohedral twin', unfortunately often used in the literature, is used even here accompanied by the hybrid monster 'merohedrical twin'. ('Merohedral' indicates a crystal whose point group is a subgroup of the holohedral group. A twin by merohedry is 'merohedric'.) Twins in staurolite are given as reflection twins, while it has been known since 1956 that they are rotation twins [see *Mineral Mag.* (1956). **31**, 145–163]. Fig. 4.A.2 is drawn from a perspective which completely hides the elbow of the 'elbow twin'. The absence of the book by Steurer and Deloudi in the literature about quasi-crystals is regrettable, but the publication schedule probably prevented insertion of this recent reference.

Chapter 5 is devoted to 'experimental methods in X-ray and neutron crystallography' and counts 92 pages plus 14 pages of appendices. This is a remarkable chapter that covers a huge range of content, from electron–matter interaction to produce X-rays to synchrotron radiation and neutron sources, detectors, equipment, data collection from single-crystal and powder samples, non-ambient measurements, data reduction, and radiation damage; the geometry of cameras has been moved to the appendices, given the historical interest this topic has today. The wealth of information could have led to a heavy text, while it is presented with clarity but without excessive brevity.

Chapter 6 presents the strategies and methods for the solution and refinement of crystal structures in 59 pages plus 29 pages of appendices. Like the preceding one, this chapter represents a comfortable journey through a complex landscape, where the traveller is guided with mastery. A complete review of the methods in direct and reciprocal space is presented (Patterson, direct methods, charge flipping, structure completion, heavy-atom method, correction of Fourier series truncation errors *etc.*). However, some considerations have regrettably been left out. Heavy atoms on extraordinary orbits do not affect the whole diffraction pattern, so their contribution to the diffracted amplitudes does not become so dominant as to make the contribution by light atoms negligible: this case should have been presented at p. 429. The whole of Appendix 6.H (*Pseudotranslational symmetry*; see also Chapter 3, p. 181, *Pseudo-translational symmetry effects*) should have been replaced and expanded with a discussion of extraordinary orbits. Again at p. 429, the need to fix one coordinate for space group $P2_1$ should have been generalized to all pyroelectric groups: the number of coordinates to be fixed varies from 1 to 3 depending on the geometric crystal class. The ambiguity in the choice of the origin touched on lightly at pp. 433 and 469 can be analysed in terms of normalizers: actually, a whole section should be devoted to this problem, which is unfortunately seldom presented, while its treatment has been well known for a long time. The absence of *JANA* in the list of software packages for least-square methods (p. 463) is difficult to accept.

Chapters 7 to 9 present the three categories of crystal structures: inorganic and mineral, molecular, and macromolecular, and span overall about 260 pages. The sequential reading of these chapters allows the reader to get precise and detailed information about the specificities of each of them and, in particular, a comparative view. This aspect could have been reinforced further if these chapters had been preceded by a short introduction where the common aspects and the difference could have been emphasized, such as the peculiar nature of inorganic and mineral crystals, for which no unit exists in the fluid corresponding to the solid state, whereas for the other structures a molecule exists in all the states of matter. This explains why a significant part of Chapter 8 is devoted to molecular features that are independent of the crystalline state and would fit perfectly in a textbook of chemistry rather than of crystallography. The short example of molecular symmetry analysis in terms of irreducible representations is unconnected to the very brief presentation given in Appendices 1.E.9 and 1.E.10; the latter, not used elsewhere, would probably have had its place here. The 65 groups with only first-kind operations, in which macromolecules crystallize (p. 697; but also Chapter 1, p. 28), are known as Sohncke groups, a term never used in the book. At p. 708 we find the strange expression 'cell length'; perhaps a shorthand for 'cell parameters' length'.

Chapter 10 ends this long excursion into the complex world of crystallography with a clear exposition of the physical properties of crystals, explained in 51 pages plus 3 pages of appendices. The new figures add value to a chapter that already in the previous edition was exempt from critics, apart from the insufficient space devoted to crystal optics; a reasonable treatment of this subject would, however, have required an significant expansion for a book that already counts more than 800 pp.

An extensive analytical index (12 pp.) helps the reader to find the topic they need.

Overall, this is not a text for beginners. To approach crystallography from scratch a more pedagogical presentation, like the classical *Crystallography and Crystal Chemistry* by Bloss (which has a much narrower target) is preferable. But once the reader has a general idea of the landscape, *Fundamentals of Crystallography* is the reference text to deepen their knowledge and understanding, despite the flaws still present in this third edition: one can hopefully expect that these will be amended in the fourth edition, when the book will finally reach its full maturity.

For an extensive text like this, the number of typographical errors is very low, which testifies to the care with which the several authors have checked their chapters.

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