



Fundamentals of X-ray Crystallography , second edition.

**By Dongcai Liang. Beijing: Science Press/Oxford:
Alpha Science International Ltd, 2011. Pp. xi + 435.
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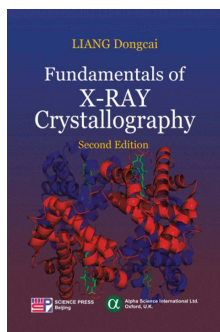
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Fundamentals of X-ray Crystallography, of which the second edition has recently been published, is the English version of a Chinese hand-

written manuscript based on the author's lectures delivered at the Department of Biology of the University of Science and Technology of China during the 1980s (the book opens with two images of pages from the original manuscript). As explained in the foreword to the first edition, the author's scientific background is in China and in the former Soviet Union, which explains why most of the references given in the book are from texts hardly known or available in the West.

The foreword to the second edition clearly states the purpose, target and approach of the book: X-ray structural analysis of biological macromolecules *via* 'simple and easily understood concepts', essentially geometrical, without any rigorous formalism. In fact, not only is the matrix formalism never mentioned, but the notion of group itself is used but never defined. This intuitive approach, far from helping the reader, makes the book quite heavy and dull, especially in the long derivation of space groups. The purely geometric description is definitely insufficient: for a book aiming at presenting 'the methods of X-ray crystal structure analysis', the complete absence of notions as fundamental as the structure factor is unforgivable. The frequent reference to 'protein' or 'macromolecular' crystallography is also unjustified: the book does not present *anything* specific to biocrystallography; it is nothing more than an introduction to geometric crystallography, with nonstandard terms and symbols, supplemented by a description of experimental techniques and equipment, adding nothing to what is available in a multitude of older texts: Laue, oscillating and rotating crystal, Weissenberg, and precession, with a short introduction to the four-circle diffractometer in Eulerian geometry.

The book, which deals exclusively with three-dimensional space without either passing through the lower dimensions or giving an insight into higher dimensions, is divided into three sections: *Fundamental Principles of Geometric Crystallography* (nine chapters, 96 pp.); *Symmetry Principle of Microscopic Space* (seven chapters, 180 pp.), and *Fundamental Principles of Crystal X-ray Diffraction* (six chapters, 133 pp.). At the end of the text we find a list of figures and a list of tables, but *no index*.

The title of the first section shows the first misunderstanding in this text: the term *geometric crystallography* is in fact used here to indicate *macroscopic* (morphological) symmetry, *i.e.* essentially point groups, as if space groups were not part of geometric crystallography too. The first chapter of this section (9 pp.) is a short introduction to the periodic nature of crystalline matter where we learn that Röntgen must have had predictive faculties because he 'discovered in 1885 that such optical gratings [crystals] could cause X-ray interference': that was ten years before he discovered the X-rays. This is just the first slip, because a few lines later we read that the atomic content of a crystal is 'abstracted into geometric points called *nodes*'. There must be some translation problem from the Chinese original, because in the following the confusion between atoms and nodes does not seem to be confirmed. However, the terminological nightmare has just started. A few lines below we find two completely different concepts – 'plane lattice' and 'lattice plane' – used as synonymous, but also pairs of different terms to indicate the same thing: 'unit lattice' and 'unit cell' (the former given as the unit of the abstract lattice, the second as the unit of the crystal structure, the two being of course identical despite the opposite statement in the text), as well as 'crystal space lattice' *versus* 'crystal lattice'; there is also a series of unusual terms like 'compound lattice' – a direct translation from the Chinese – to indicate a centred lattice, and 'space grid' to indicate a three-dimensional lattice. [It should be noted that the expression 'centred lattice' is itself awkward, being short for 'lattice whose conventional cell is centred'. See S. F. A. Kettle & L. J. Norrby (1993), *J. Chem. Educ.* **70**, 959–963.] A surprising expression follows: 'either the shape or the internal structure of a crystal has unique symmetry that is defined by the internal structure of that crystal': how one of the two symmetries could not be determined by the internal structure is not explained. The chapter ends with another strange expression, 'transition phase' (certainly a wrong translation for 'phase transition') and a too absolute statement according to which 'a crystalline state is a thermodynamically stable state that cannot be spontaneously transformed into other phases unless an external event intervenes': diamond salesmen are certainly most happy that this statement is incorrect.

Chapter 2 is a very brief (6 pp.) introduction to the law of the constancy of interfacial angles, optical goniometers and the gnomonic and stereographic projections. The expression 'isomorphic crystals' is incorrectly used to indicate two crystals of the same compound which have developed the same crystal form (the latter being never defined). Figure 1-2-4 shows axes ρ and ψ , but the text discusses an axis φ which does not appear in the figure.

The third chapter (20 pp.) introduces morphological symmetry and types of symmetry elements *via* the stereographic projection. The 'symmetry graph' in Figure 1-3-1, which should present the identity operation, is identical to that in Figure 1-3-2, which presents the inversion. Symmetry planes (mirrors) are drawn as double lines and twofold rotation axes are drawn as black ovals inclined at 45° to the left, and this throughout the whole book. The symbol for the $\bar{4}$ axis in Figure 1-3-13 is given in its negative image: a white oval within a black square, instead of the opposite: the same mistake occurs in Figures 1-4-11, 1-5-8 and 2-3-8, whereas, strangely enough, it is correct in the following figures (Figures 2-4-4, 2-4-5, 2-4-6, 2-6-22 and 2-6-25).

The combination of symmetry operations (called 'elements') is presented in Chapter 4 (13 pp.), where the concept of a point group is used without having being defined. White ovals are used for twofold rotation axes parallel to the direction of projection, while black ones are used for axes in the plane of projection. The orientation of the hexagonal axes is not standard (rotated 30° counterclockwise with respect to the standard orientation) in Figures 1-4-9, 1-4-10 and 1-4-15 but not in Figures 1-4-12 and 1-4-13: the different choice is not explained.

Chapter 5 (11 pp.) introduces 'symmetry combinations allowed in crystals', *i.e.* crystallographic point groups: only morphology is presented; the symmetry of physical properties is not even mentioned. The set of symmetry operations is called the 'symmetry transformation group', whereas the set of symmetry elements is called the 'symmetry element group': the latter is obviously nonsense, geometric elements about which operations are performed do not form a group, while the operations do. But, as we have already remarked, the concept of a group is never defined, so it is not impossible that in this book the term is used in a loose way to indicate a set of objects. A totally personal way of classifying 'symmetry combinations' (point groups) is presented, in five 'categories' (A to E), on the basis of the number of symmetry elements: pyroelectric groups (a term never mentioned, replaced by 'category A'), twofold axes perpendicular to the polar direction of pyroelectric groups ('category B'), mirrors containing the polar direction of pyroelectric groups ('category C'), a mirror perpendicular to the polar direction of pyroelectric groups ('category D'), and mutually perpendicular mirrors ('category E'). A purely geometric derivation of point groups in terms of the mutual orientations of the symmetry elements is presented, with the 'coordinates' *xyz* of stereographic poles given instead of the Miller indices – the latter term being never mentioned in the book.

Chapter 6 (9 pp.) introduces the crystallographic axial settings and the notion of the crystal system. As in a number of other texts, the term *crystal system* and the criteria for defining it, namely the relations between the parameters of the conventional cell, do not match: what is presented here is the set of *lattice systems*, not the crystal systems. Another common mistake, in Table 1-6-1 and in the rest of the text: relations among cell parameters which are not imposed by the symmetry. For example, the cell parameters of the triclinic lattice system can take *any* value and are not symmetry

constrained to be different: therefore, to write $a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^\circ$ is imprecise. The same holds all the other lattice systems with the exception of the cubic one, the only system where the size of the unit cell is the only freedom left by the symmetry constraints. Table 1-6-1 also presents a strange classification into three categories called the 'lower crystal system', the 'intermediate crystal system' and the 'higher crystal system': these correspond to the well known classification of biaxial, uniaxial and isotropic crystals in crystal optics. The use of personalized terms to replace standard ones is unjustified and unacceptable. The same can be said for the expression 'all-symmetric type point group' instead of holohedry. This short introduction ends with the first piece of information (one of the very few) specific to biocrystallography: the limited number of point groups in which macromolecules crystallize: certainly insufficient to qualify the text as specifically devoted to biocrystallography.

Chapter 7 (8 pp.) introduces 'crystal face indices' (*i.e.* the Miller indices) and indices of rational directions (called 'crystal edge indices'); it contains a couple of typographical errors and ends with an octant of the stereographic projection of a cubic crystal, without any explanation: incomprehensible for a beginner.

Chapter 8 (16 pp.) introduces 'the equivalent point set' defined as 'a symmetrically equivalent point': probably another direct translation from the Chinese? A bad confusion between 'set' and 'group' appears at p. 79, when the two terms are used interchangeably. But much worse is the confusion between the coordinates of a point and the indices of a face or plane, which leads to the appearance, in the stereographic projection in Figure 1-8-1 of a pole at the centre of the sphere! The same type of slip occurs in Table 1-8-1, where the orientation of point-group symbols with respect to symmetry directions is also given for the triclinic system, where a phantom direction [000] appears: how the origin alone could define a direction is a mystery. Another nonsensical statement appears just below the table, when we read that 'In point group *mm*2, the normals to the symmetry planes and the 2-fold axis are equivalent.'

Chapter 9 (4 pp.) introduces 'monomorphous crystal forms' and 'composite crystal forms' and is again a terminological nightmare. First of all, the term *form*, never defined, is used for 'morphology' (external shape, developed faces). Then 'monomorphous' and 'composite' are used to indicate a crystal composed by only one form (the real one, not what is meant in this book) or by more than one form, respectively. The icing on the cake is the use of 'Wyckoff set' in place of the standard term 'form'; let us add that in crystallography the term 'Wyckoff set' has a precise meaning (set of Wyckoff positions conjugated in the normalizer) and the confusion reaches its apogee. But this short chapter has still some surprises to disclose. Page 97 states that 'there are 47 monomorphous crystal forms [...] each [...] has a specific name in geometric crystallography.' This statement identifies the 'monomorphous crystal forms' with the true forms (contradicting the definition) and implicitly states that each (true) form can compose a crystal, which is impossible for all open forms.

The second section is a long and tiresome descriptive derivation of space groups, without group-theory tools but using just combinations of motions. If the purpose of this section is to exhaust even the bravest reader, then its goal is certainly achieved. Otherwise, the 180 pages of this section could have been used in a much more profitable way to help the reader to understand *International Tables for Crystallography*, instead of taking them wandering through a desert to arrive at some confused ideas which are presented in a much clearer and complete way in countless other texts. The interest of this section is especially questionable for protein crystallographers, who are the explicit target of the book.

Chapter 1 (8 pp.) is devoted to ‘translation in microscopic space’ and introduces two axial settings, *abc* and *XYZ*, which are constrained to coincide. Besides a few typographical errors and some sentences that are hard to understand, we find the ‘first kind’ and ‘second kind’ of unit cells, for primitive and centred cells, respectively. The rhombohedral centring is absent.

Chapter 2 (14 pp.) introduces screw axes and glide planes. It is to be noted that the *e* glide is absent: for a text published in 2011, this further departure from the IUCr standards is incomprehensible.

Chapter 3 (18 pp.) is devoted to obtaining graphically the result of the combination of the symmetry elements introduced in the previous chapter with translations. The caption of Figure 2-3-1 exchanges reflections for inversions. On p. 132 we find an ‘*H* unit cell’ which should correspond to the *hP* cell: the mistake is not venial, because in crystallography an *H* cell (more correctly indicated as *hH*) does exist: it is a triple cell containing centring nodes at $1/3, 2/3, 0$ and $2/3, 1/3, 0$.

Chapter 4 (41 pp.) is a long and tedious graphical derivation of space groups as a combination of motions, not always with the necessary change of origin to arrive at the standard description. It should be noted that, at this point, Bravais lattices have not been introduced! The graphical symbol for a horizontal *n* glide lacks an arrowhead. The comma to indicate a change of chirality in the space-group diagrams is sometimes present, sometimes absent. Figure 2-4-14 shows mirrors of type *g*, which are incorrectly called *a*.

Chapter 5 (25 pp.) finally presents Bravais lattices, as introduced by a certain O. Bravais in 1895 (instead of Auguste Bravais in 1850). This chapter is full of misunderstanding and confusion. We read that ‘any nonprimitive cell is not a Bravais cell in the triclinic crystal system’ (p. 186). Apart from the fact that the term ‘Bravais cell’ is not standard, it goes without saying that any cell describes a Bravais lattice, and this is especially true in the triclinic system where there are no symmetry constraints in the choice of the cell. We then discover that the conventional choice of the *b* axis as the unique monoclinic axis is the *only* possibility, instead of a matter of convention, and that *I* and *F* monoclinic cells are ‘not correct’, instead of being simply unconventional. The rhombohedral cell is given in the reverse setting only, and an unconventional *I*-centred rhombohedral cell is also introduced which is the reverse *hR* cell with double period along the $[111]$ rhombohedral direction; the standard observe setting is

mentioned in passing on p. 197. For the hexagonal lattice, the set of three hexagonal primitive cells forming a *C*-centred hexagonal prism corresponding to a triple cell is used, while the standard primitive cell is described as ‘representative of the partial *H* lattice’ (p. 204): what a partial lattice could be and how a primitive cell could represent only a part of what is represented by a centred cell remains another mystery in the crystallographic cloud covering this chapter. The orthorhombic cell is also introduced for both the hexagonal and rhombohedral lattice, without giving, however, the metric constraints ($a = b \times 3^{1/2}$ or $b = a \times 3^{1/2}$). The priority of $\bar{3}$ over 3 in rhombohedral and cubic space groups is not respected.

Chapter 6 (31 pp.) introduces space groups as ‘combinations of microscopic symmetry elements and nonprimitive translations’. The *d* glide is described as having ‘special features’ but the fact these come from the choice of a centred cell should have been explained.

Chapter 7 (44 pp.) tries to obtain all types of space group by combining types of lattices and point groups, and adding nonprimitive translations. Only eight figures are given for 230 types of space group, the derivation consisting essentially of text. A series of seven criteria for choosing the origin is given: had the elementary notion of a site-symmetry group been introduced, much of the cumbersome mechanism would have been avoided. The sentence ‘in the orthorhombic crystal system, there is more flexibility in the choice of the unit lattice [read: unit cell] than in the triclinic and monoclinic crystal systems’ (p. 247) can hardly be attributed to a bad translation but looks like a fundamental mistake, whose origin is difficult to grasp. A long discussion about the transformation of orthorhombic space-group symbols follows: this would have been much more useful if applied to axial settings differing not only by a permutation of the axes – for example, the tetragonal expression of an orthorhombic space group, quite useful in the study of possible phase transitions. When the third element in the point- or space-group symbol is not a generator, only two symbols are used, as in the old editions of *International Tables* (*International Tables for X-ray Crystallography*, the ‘red books’): one more departure from the international standards. The derivation of the Wyckoff positions (called ‘equivalent point systems’) is presented for the space-group type *Ama2*, without projection of the atomic positions.

The last section introduces X-ray diffraction. Chapter 1 (6 pp.) describes X-rays. Chapter 2 (12 pp.) introduces the reciprocal lattice and contains several problematic statements. First of all, reciprocal space is defined as ‘not a real physical space’: it would have been useful to have a definition of what is meant to be ‘real’ and ‘physical’ in this book, because given we do see and record diffraction effects, it is difficult to accept them as something ‘not real’ (a dream? an illusion?). For the construction of the reciprocal lattice, up to *seven* basis vectors are used, namely for centred lattices. It should be obvious that in a three-dimensional space three independent vectors are always enough: the problem here comes from a confusion in the definition of Miller indices and interplanar distances – a confusion that was present in Friedel too (*Leçons de cristallographie*, 1926, pp. 234–245) but that, to the best of our

knowledge, has never occurred since. In this chapter, and especially in the following one (17 pp.), the concept of integral reflection conditions is introduced by changing the value of the interplanar distances $d(hkl)$ as a function of the type of centring, instead of making a choice of Miller indices consistent with the definition. For example, in the case of a two-dimensional lattice whose conventional cell is *c*-centred ('*oc* lattice') the (10) and (01) family of planes are retained but the interplanar distance is given as $a/2$ and $b/2$, leading to an 'incomplete reciprocal lattice' (p. 306). Quite obviously, for an *oc* cell these families are (20) and (02) (the first plane of the family cuts both *a* and *b* at $\frac{1}{2}$), the calculation of $d(hkl)$ is not modified, and the absence of 10 and 01 reciprocal-lattice nodes is a direct consequence of the consistent choice of Miller indices. The concept of 'incomplete reciprocal lattice' is clearly nonsense, because a primitive reciprocal cell describes the same lattice as 'complete': it is the *description* of the lattice by a bigger (centred) cell in direct space which leads to a smaller cell in reciprocal space. The reader's headache reaches its climax at p. 317, when they have to face a statement according to which a reciprocal unit cell does not represent a lattice, for which one needs a set of unit cells which form a 'reciprocal lattice unit' which is 'neither a reciprocal unit cell nor a unit reciprocal cell'.

Chapter 4 (16 pp.) introduces geometrical diffraction (the Laue and Bragg equations) but ends with an astonishing statement according to which 'any complicated structure can always be divided into certain simple structures that are parallel and overlap each other' so that 'the complicated structure [...] generates diffraction in the same condition as that of the simple structures'. In other words, and unless a macroscopic translation mistake from the Chinese has occurred, this text considers only structures built by atoms occupying the same type of Wyckoff positions and ignores all the others.

Chapter 5 (42 pp.) deals with 'the diffraction sphere and diffraction space', the former being of course Ewald's sphere (never mentioned by its name), but actually introduces the bulk of geometrical diffraction. Indeed, the intensities are never considered in this book but only mentioned without any definition or formula. Nonetheless, the 'anomalous diffraction effect' is mentioned a few times from p. 345: how the reader could guess what this is without having been introduced to the scattering power of atoms and the structure factor remains a (another) mystery. Zonal and serial systematic absences are introduced again as an absence of lattice *nodes* instead of lattice nodes associated with zero intensity: the concept of a weighted reciprocal lattice should be mandatory to avoid this type of misunderstanding. Diffraction symbols occupy a long table which is essentially a copy of what we find in Part 4 of Volume A of *International Tables for Crystallography*. The chapter ends with a derivation of the equivalence of diffractions in the 11 Laue classes and a few considerations of beam divergence and line width. The meaning of 'equivalence' without the notion of the structure factor is questionable. The derivation proceeds *via* group-subgroup relations, from $6/mmm$, $m\bar{3}$ and $m\bar{3}m$: the need to treat $m\bar{3}$ separately, when it is a subgroup of $m\bar{3}m$, is a further mystery.

Chapter 6 (40 pp.) deals with single-crystal diffraction methods: Laue, oscillating crystal, rotating crystal, Weissenberg and precession, with a short presentation of four-circle diffractometry. While it is true that these techniques have experienced a renaissance for protein crystallography at synchrotron facilities, the description is entirely classical and highly reminiscent of old books.

Several awkward or nonstandard expressions are disseminated throughout the text, most likely coming from an imperfect translation from the Chinese: 'lattice surface' instead of 'lattice plane' (pp. 12–13); 'lattice properties' instead of 'periodic properties' (p. 12); 'polar points' instead of 'spherical poles' (p. 15); 'reticulate' instead of 'reticular' (p. 62 and following). On p. 19 the expression 'circular projection sphere' tantalizes the reader with the possibility of a sphere that would not be 'circular'. 'Independent symmetry elements' and 'derived symmetry elements' are used instead of 'generators' and 'generated symmetry elements' (p. 91). The almost unbelievable term 'nonhigh-fold axis' for 'twofold axis' appears on p. 123. The mystery of a '2-dimensional direction' occurs on p. 141, while the following page introduces the almost esoteric term 'symmetry equivalent points of the symmetry element'. On p. 148 we find the adjective 'imaginary' added to 'inversion point' of an even-fold inversion axis. A 'general discussion' is declared on p. 152, which instead proceeds with one example. The 'principle of microscopic symmetry' is used from p. 155 on, and the 'macroscopic symmetry principles' from p. 164, but neither is ever defined. Friedel's law (a term which is never mentioned) is defined by the statement 'the diffraction sphere is always centrosymmetric' (p. 346). 'Symmetry operative translation' is a pleonasm occurring on p. 349.

Several typographical errors ('plan' for 'plane'; 'it's' for 'its'; 'nonpreliminary' for 'nonprimitive'; nine orthorhombic Bravais lattices instead of four) occur here and there in the text, while Figure 2-6-13 shows a wrong glide direction for the d glide at $\frac{1}{2}yz$.

In summary, this book covers part of the content offered by Buerger's classical textbooks *Elementary Crystallography* and *X-ray Crystallography*, published in 1956 and 1942, respectively, which are much more rigorous, better and more clearly written, close to the international standards, and complete, with the only exception being the introduction to the four-circle diffractometer, which, however, occupies only two pages. The original Chinese may have some interest for native speakers less confident with the English language. Publishing an English translation is instead completely unjustified: it gives the reader the false impression that almost nothing has happened since Buerger's time. While it does not contain catastrophic errors, it creates a lot of confusion by using non-standard terms, symbols and descriptions, and contains some questionable statements, to say the least. Another book to be forgotten.

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