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Massimo Nespolo

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# Foundations of Crystallography

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# Massimo Nespolo

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### book reviews

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## book reviews

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**Crystallography and the World of Symmetry.** By Sanat K. Chatterjee. **Springer Series in Materials Sciences**, No. 113. Springer, 2008. Pp. xi + 150. Price (hardback) GBP 87.00. ISBN 978-3-540-69898-2.

The International Union of Crystallography produces a number of books on crystallography in association with Oxford University Press and Springer. When a book on crystallography is published independently, outside the framework of the IUCr, this should in principle be welcomed as a sign of dynamism of our discipline showing its true character as an interdisciplinary science. This particular book, however, does not warrant such a welcome.

Crystallography and the World of Symmetry is a thin book (only 150 pages including exercises and the analytical index) with a clear didactic purpose at the undergraduate level. A book of this kind can be conceived in two ways: as a textbook to be read by the students, or as a reference for the lecturers. Crystallography and the World of Symmetry does not fit either category: it fails in both respects.

Crystallography and the World of Symmetry consists of three parts: geometrical crystallography (Chapters 1–5), experimental methods (Chapters 6–8) and a more general excursion about symmetry (Chapters 9 and 10), followed by a two-page epilogue, two appendices and suggestions for further reading. Before analysing the content, one cannot refrain from stressing that, with only one exception mentioned below, no reference is made to *International Tables for Crystallography*, which is not even listed in the *Further reading* section: in a book on crystallography this is at least surprising. We will see that actually this missing reference is perhaps the least surprising fact about this book.

Chapters 1-5 (pp. 1-42) aim to provide the reader with some basis in geometrical crystallography. This part contains several serious mistakes and misunderstandings. Chapter 1 rapidly introduces the concept of a periodic pattern as a regular repetition of an object called a 'motif', a questionable choice because 'motif' is simply the French term for pattern. The definition of a lattice as 'the sites of motifs where they can be placed to generate the pattern' (p. 6) is the first blunder in this book, because it implicitly restricts the atomic positions (positions of the 'motifs') to coincide with the lattice nodes, a mistake that occurs again in the following. Chapter 2 presents a bird's-eye view of two- and three-dimensional lattices. On p. 13 we learn that the {110} family of planes comprises six planes in general, i.e. without any reference to the symmetry of the crystal. We also read that these planes 'belong to the same class'. A few lines below we discover that the [uvw] indices of lattice directions are called 'Miller indices'. These can, however, be considered as minor errors. Where things start

getting serious is in Chapter 3, in which Symmetry in Lattices is approached and where Hermann-Mauguin symbols are used without being introduced or explained. Even before entering the body of the subject we read that 'the symmetry in the lattice is the *minimum* symmetry present'. The axes of rotations in Fig. 3.2 are applied to two-dimensional figures with the exception of the fourfold axis, which is applied to a cube: the reason for this heterogeneity is unclear. Fig. 3.4 should show the four mirror lines (incorrectly called 'planes') in a tetragonal two-dimensional lattice; however, the diagonal lines pass close to but outside the lattice nodes. This can be considered one of the many imperfections of the drawings in this book. Not just a printing problem but a real mistake appears in Fig. 3.5, where a two-dimensional pattern is shown with a diagonal line which should be a mirror but which passes through objects not having the corresponding eigensymmetry. Worse is the case of Fig. 3.6, where an irregular polygon (in two dimensions: not a polyhedron in three dimensions) is described as possessing 'a centre of symmetry at the point P', which is the centre of the polygon. Any possible doubt about the interpretation of this is removed when reading §3.1.3, where it is stated that 'The unit cells of all plane lattices have a centre of symmetry'. The concept is again repeated in the following page, where it is stated that 'The onefold rotoinversion (1) ... may exist on a plane'. What is described here is simply a twofold rotation, as a centre of symmetry does not exist in even-dimensional spaces. Finally, Fig. 3.8 should show the equivalence between  $\bar{2}$  and m but the arrows used as the objects on which the operations act would not overlap when one of them is reflected by the mirror: just one of the many typographical problems in this book.

Crystal symmetry is introduced in Chapters 4 and 5. Symmetry elements without and with a gliding component are called 'macroscopic' and 'microscopic', respectively, something that indirectly could suggest to the reader that the former are not present in the structure. On p. 23, a point group is described as 'that collection of macroscopic symmetry elements which occurs at every lattice point'. The difference between the point group and site-symmetry groups, which act in two dual spaces, is absent: a sort of average of the two concepts is presented instead. The footnote to a table of the 32 types of point groups in three-dimensional space (pp. 24–26) states that 'No. 32' (the cubic holohedral group) 'is the most highly symmetrical all of the point groups of symmetry'. What is probably meant is that this group is the one with the highest order (the concept of order of a group being, however, absent in this book), because otherwise the statement is wrong, given that the hexagonal groups are not subgroups of the cubic holohedry. Table 4.2 repeats a typical mistake present also in many other texts: it presents the seven crystal systems as if

they were uniquely characterized by the lattice parameters, i.e. the classical confusion between crystal system and lattice system, which is confirmed by the use of 'rhombohedral' as a synonym of 'trigonal': this mistake is deeply rooted in the French literature because of historical and linguistic reasons, but one does not expect to see it appearing in an English text. The misunderstanding is further compounded on p. 32, where some examples of substances crystallizing in the various 'crystal systems' are listed and where we discover that quartz would be rhombohedral, instead of having a hexagonal lattice (the space group of low quartz is  $P3_121$  or  $P3_221$ ). The confusion becomes even greater when (in §4.3) it is stated that crystal systems 'sometimes are also named as crystal classes'. Section 4.4 shows six types of lattice centrings in which R is missing: this is not surprising, given that the R centring occurs in the hexagonal crystal family but instead here the rhombohedral lattice is treated as if it were a crystal system. Furthermore, in Fig. 4.4 the possible centrings of a rhombohedral lattice are analysed and the conclusion that the lattice is again rhombohedral is reached, something that is self-evident as the rhombohedral lattice is a centring of the hexagonal lattice. Table 4.5 shows the 'redundant space lattices', i.e. the different centrings that are not independent in each 'crystal system'. Here we discover with great surprise that A, B and C centrings in cubic lattices as well as A and B centrings in tetragonal lattices are 'redundant', instead of being incompatible with the lattice symmetry. The icing on the cake of this chapter is contained in the two expressions 'The number of lattice points, N (atoms or molecules in actual crystals)' on p. 32 and 'A primitive cubic lattice unit cell has atoms at the corner', p. 33, where we understand that in this book a lattice node and an atom are treated as being the same.

Chapter 5 contains some discussion of space groups and arrives at the conclusion that space groups 'can be derived from the group theory and geometrically' but it is 'cumbersome', and only an example of combining lattice centrings and symmetry elements for a monoclinic crystal is given. Turning a blind eye to the statement that screw axes and glide planes (called 'microscopic symmetry elements') 'can *only* be identified by the study of the internal arrangement of the motifs' (the Bravais–Donnay–Harker law notwithstanding), at p. 40 we discover the existence of '230 types of crystal space *lattices*'.

After this nightmare journey in direct space, we approach the land of X-ray diffraction and experimental techniques where, however, other problems await us. Chapter 6 is the calm before the storm: we travel relatively safely across a brief account of the production of X-rays, a glimpse at Bragg's law (12 lines) and an axiomatic introduction to the reciprocal lattice and Ewald's sphere, with some computations of  $d_{(hkl)}$ . We land finally at Chapter 7, where experimental methods are presented. Which experimental methods can be expected in a book on crystallography published in 2008? Of course, Laue, Weissenberg, de Jong–Boumann, precession and Debye–Scherrer cameras and rotation/oscillation photography. Single-crystal diffractometry is probably outside the scope of the book, let alone synchrotron radiation, later mentioned once in passing (p. 123). In this chapter we learn to use Bernal

charts (erroneously called Barnal charts) to index rotatingcrystal photographs and Weissenberg charts for the homonymous photographs, the use of a precision (occurring four times, even in the analytical index) instead of precession camera is described and we learn that a powder sample is a 'polycrystal' characterized by grain boundaries while a single crystal has a long-range order 'extended all through the bulk'. We then encounter the section on the Debye-Scherrer Cylindrical Powder Camera, perhaps the only example ever of a text beginning with an equation, which naturally leads to the indexing of the Debye-Scherrer pattern, where we discover the existence of four cubic lattice types (the diamond structure is here mistaken for a lattice, despite its absence in the table of lattice types in Chapter 4). Suddenly, we have to face the missing of some lines 'because of zero structure factor', the latter being an entity not defined or explained but used again on pp. 80-81; it is introduced in Appendix A, which is, however, never referenced.

Chapter 8 introduces methods for the determination of space group and crystal structure, i.e. trial-and-error methods and the Patterson function: direct methods (let alone charge flipping) are not even mentioned. First of all, the determination of the space group from Weissenberg photographs is briefly described and some calculations of structure factors are carried out to introduce some examples of systematic absences; for a complete list of these International Tables is here mentioned for the first and only time, but Volume I is quoted (the 1952 edition, one assumes: no reference is given). The section on the trial-and-error method ends with a paragraph discussing the Patterson function, which should have been put in the next section. However, on reading that section one can find no place where this displaced paragraph would fit: it probably results from an error in copying and pasting from a previous version of the manuscript.

Chapter 9 starts the third part of this book, where a general semi-philosophical description of symmetry in Nature is presented. Even in this chapter of general nature we find serious mistakes: Fig. 9.8 shows two Egyptian two-dimensional patterns in which we are told a 4 axis is present, in striking contradiction with the previous statement (p. 20) that in a plane no 'higher roto-inversion axis' may exist (we have already seen a twofold rotation in the plane mistaken for an inversion centre). The reasoning gets more philosophical when fundamental particles and anti-particles are compared and considered pairs of 'reflected images' across a mirror plane that divides matter and antimatter. The chapter ends with some arguments about the invariance of physical laws and shows the effect of a mirror reflection on a force  $\mathbf{F} = \mathbf{r} \times \mathbf{p}$ , where a particle on one side of the mirror rotates left and the corresponding particle on the other side of the mirror rotates ... again left!

Chapter 10 deals with Asymmetry in Otherwise Symmetrical Matter. Once again, a single crystal is presented as a homogeneous object without grain boundaries. The concept of a stacking fault is introduced through Burgers vectors, which are never defined. Section 10.2 introduces quasicrystals: here the term 'compact' is used instead of 'periodic' (one wonders why)

### book reviews

and once again the atomic positions, this time in the framework of a Penrose tiling, are restricted to the *vertices*: the idea that an atom may take a position *within* a unit cell seems unacceptable. Section 10.3 introduces liquid crystals. The optical study of these materials by the polarizing microscope is presented in less than two pages. Section 10.4 challenges the realm of nanostructures. A brief description of fullerenes is followed by a paragraph starting with 'These tiny tubes of carbon ...': we have moved from fullerenes to carbon nanotubes but at least one connecting paragraph has been lost. On p. 123 we discover that diamond has 'molecular bonds', on the basis of which one would have serious problems explaining its properties.

The final pages, after a philosophical epilogue, give a very short account of diffraction theory (Appendix A) and a few solved exercises on lattices and on the calculation of systematic absences, where we discover that NaCl is two f.c.c. lattices; quite obviously, the lattice of NaCl is one, but the cations and the anions form two lattice complexes.

The number of typographical errors, mistakes in the English and problems in the figures suggest that no proof corrections have been made. Some examples: in the table on p. 24 we see a strange group '2/s'; Figs. 5.4, 9.4 and 10.16 are black and white, but their captions indicate the presence of colour; Fig. 10.4c shows an SEM image, not an electron diffraction micrograph as stated in the caption; Fig. 10.6 has a top and bottom part (on pp. 109 and 110, respectively), not a left and right part as stated in the caption; p. 123 refers to Fig. 10.9 about aggregated carbon nanorods, while this figure in fact shows a scheme about liquid crystals: the correct figure is missing.

We can conclude our analysis by saying that this book was probably published without a full review process, otherwise *at least* the serious problems in the figures, the internal contradictions of the text and the missing or displaced parts of text would have been noticed. What, however, remains most incomprehensible is how such a text, full of mistakes, misunderstandings and serious blunders, could have been published. Having appeared in a book series, it is automatically acquired by subscribing libraries all over the world and is easily accessible to a large body of scientists (we have to keep our fingers crossed that it does not end up in the hands of some students) who will hardly believe their eyes when reading the text.

Can we find any positive consequence from the publication of this book? In a certain respect we can: this book is a paradigmatic example of the dramatic consequences that the lack of serious crystallographic education may have. Teaching crystallography is constantly decreasing in our universities: crystallography courses are being axed or have to disguise themselves within more general titles of, say, physics or material sciences. To convince the authorities that a serious education in crystallography is absolutely necessary, we can show them this book as a perfect example of the damage that results when crystallography is not taught and understood.

#### Massimo Nespolo

CRM2 UMR-CNRS 7036 Institut Jean Barriol Nancy-Université BP 70239 F-54506 Vandoeuvre-lès-Nancy cedex France