

## Review of

Jakub Plášil, Juraj Majzlan and Sergey Krivovichev (eds.) (2017) **Mineralogical Crystallography**. EMU Notes in Mineralogy, Vol. 19, European Mineralogical Union and Mineralogical Society of Great Britain and Ireland: London. ISBN 978-0-903059-5, X, 258 p., £ 55.00 (institutions) £ 40.00 (individuals)

MASSIMO NESPOLO, Université de Lorraine, CNRS, CRM2, Nancy, France – [massimo.nespolo@univ-lorraine.fr](mailto:massimo.nespolo@univ-lorraine.fr)

Crystallography originated from mineralogy and mineralogy could not have evolved from an empirical discipline to a comprehensive science without the mathematical and atomistic approach characteristic of crystallography. Yet, in many university curricula mineralogical crystallography is a shrinking intersection domain, like the end stage of a mitosis generating the two heterozygous disciplines. Indeed, with mineralogy trying to mutate in order to survive in a fashion-driven world which tends to consider it a heritage of the past, and crystallography victim of the success of automatic equipments and software packages, mineralogical crystallography does not get much of the spotlight. Reactions against this forgetfulness are ignited by the Special Interest Group No. 5 *Mineral and Inorganic Crystallography* of the European Crystallographic Association and of the Commission on Inorganic and Mineral Structures of the International Union of Crystallography, and signs of a renewed interest are arising. Among these, two special issues dedicated to the topic (*Zeitschrift für Kristallographie*, in press, *Acta Crystallographica* Section B, in preparation), a recent volume published by DeGruyter (Armbruster & Danisi, 2015) and Volume No. 19 of the *EMU Notes in Mineralogy*, reviewed here.

Because it is impossible to extensively cover the wide diversity of the field in a single volume (an encyclopedia would be required), the editors had to choose some aspects to put in the foreground. The result is however quite skewed towards what can be considered “hot topics”, leaving outside most of the classical content which probably still represents the bulk of the investigation in the field.

The first chapter (seventy-seven pages), authored by Sergey V. Krivovichev, deals with “Structure description, interpretation and classification of structural mineralogy”. The author is a world authority in the analysis and classification of inorganic and mineral structures in terms of complexity and hierarchy, and his chapter is a journey into a large number of families of minerals which grants the reader a key to understand how Nature plays Lego, obtaining an impressive variety of structures from a relatively limited number of building blocks. However, this chapter is practically a reprint of an article appeared the same year (Krivovichev, 2017); a typo and a missing reference here but not there suggest that the manuscript might have been sent to this volume first. This does not reduce, obviously, the scientific value of the contribution, but the reader will not find anything more or new with respect to the journal article. We regret that polytypism gets only five lines and that no mention is done of Takéuchi’s (1997) concept of trochocemical cell-twinning, despite its prominent role in the section about homologous series (Fig. 45 and 46 in particular). We also notice that Bond Valence still gets emphasis while more modern and efficient approaches like the Effective Coordination Number (ECoN) and the Charge Distribution (Hoppe, 1979; Nespolo, 2016) are completely ignored. Apart from this, and the use of “space group” when instead reference is clearly made to the *type* of space group, the reader has certainly much to learn from an attentive study of the chapter.

The second chapter (fifty-nine pages), authored by two Italian groups from Bari and Milano, presents powder X-ray diffraction. The topic is clearly of paramount importance for many investigators and can be a sort of trap; the authors did not fall in it but avoided giving the same basic notions one can easily find in countless textbooks and review articles. The reader will not find a derivation of Bragg’s law or Ewald sphere, nor will he/she learn about interaction of X-ray with matter; this knowledge is assumed to be in the background of the reader. The chapter instead very much addresses how to extract information from a powder X-ray pattern. After a general description of what a powder pattern looks like and what type of information one can get from it, the problems one most commonly faces are briefly but clearly presented (peak overlap, background, preferred orientation), followed by two sections on qualitative (“what’s in your sample”) and quantitative (“how much of each component”) analysis: approaches, methods, techniques and (some) software. This is followed by a whole section on structure solution (indexing, space-group determination, extraction of the information from peak positions and intensities), and strategies for structure refinement. The distortion of polyhedra are evaluated by various parameters, yet one of the most efficient, ECoN, is again ignored. The Rietveld refinement gets only slightly more than one page: considering its widespread use, it would probably have deserved some more details. The chapter ends with an excursion at extreme conditions (actually, only temperature and pressure; nothing about samples under electric field or about photocrystallography, for example) including a too short comparison with neutron powder diffraction and a case study about a zeolite. If on one side the authors deserves kudos for the slim and efficient presentation of the methods without wasting time and space in repeating what is available in so many other texts, they also deserve serious criticism for the sloppy and incorrect language which renders the reading disturbing and fastidious. One wonders what “number of molecules” and “molecular weight” (page 98) have to do with minerals, which are eminently non-molecular (with a few exceptions); the general terms “number of formula units” and “formula weight” should have been used instead. The *hkl* integers by which a diffraction pattern is indexed are incorrectly treated as Miller indices of lattice planes, instead of Laue indices of diffractions (page 101). The term “elementary cell” is a direct translation from the Italian and is improperly used, because the unit cell obtained by the indexing procedure can well be a multiple (centred) cell, not primitive (thus, not “elementary”; page 101 again). Table 1 presents the reciprocal of the square of the interplanar distances (thus, the square of the norm of the reciprocal lattice vector) as a function of the Miller indices, for crystal *families*, not for crystal *systems*, as incorrectly stated in the table heading (page 103). The reflection conditions are incorrectly called “extinction conditions” (page 104; extinction is a physically completely different phenomenon). Phonons are called “lattice vibrations” (page 114), which

is clearly meaningless, the lattice being a mathematical description of the periodicity of the structure; what is vibrating are atoms. The description of the way to choose the candidate space group given at page 105 does not seem correct. Here the lowest symmetry group compatible with the extinction symbol is retained, its supergroups are considered only if this one fails. However, the same structure can be described in a subgroup, but not in a supergroup: the fact that solution does not fail in a subgroup is no guarantee that it is not more symmetric, whereas if the solution fails in a supergroup, it is safe enough to assume that the structure is less symmetric. A more venial sin is the redundancy of names for the same object: “unit-cell constants”, “cell parameters”, “lattice parameters”... chose one and stick to it! (The second one is certainly the most appropriate, by the way). One may also wonder why authors felt the need to specify “inter-tetrahedral” rotation (page 126; can we have an “intra-tetrahedral” rotation?). It is really a pity that the quality of the chapter content is affected by its defective presentation.

The third chapter (forty-three pages) is devoted to electron crystallography and is the output of a Czech-Italian cooperation. It shares with the previous chapter the approach aiming at leading to reader to understand how the methods and techniques work and what information can be obtained from them, rather than a lengthy theoretical introduction already available elsewhere. After a brief introduction to the interaction of electrons with matter (one wonders why cathodoluminescence and Auger electrons are not mentioned at all), about half of the chapter is devoted to the techniques (TEM, electron diffraction) with much emphasis on Convergent Beam and Precession electron diffraction: a choice much appreciated, considering that it is not easy to find a clear but concise treatment of these techniques (often just mentioned, or otherwise treated with such a mathematical in-depth to discourage the end user). The second part is devoted to applications, in particular to structure solution and refinement, made possible in particular by the precession method and electron diffraction tomography. Sure, the quality of the refinement has clear limits with respect to that obtained by X-ray diffraction, but the size of the sample for which such a quality of refinement can be obtained is also much different. The authors have to be praised for giving credit to the Russian school (Vainshtein, Zvyagin), which introduced the Oblique Texture Electron Diffraction, in some respects the ancestor of the precession method; this is too often ignored in similar texts. The chapter is overall very well written, with however some slips, like “axial” (instead of serial) reflection conditions (page 162), symmetry “operators” (instead of elements; page 164), a 6-layer polymorph instead of polytype, with polytypism called “stacking polymorphism” (page 166). As in the previous chapter, “unit-cell parameters” and “lattice parameters” are used in alternating way.

The fourth chapter is the shortest one (twenty-nine pages). Authored by F.M. Michel, it presents total scattering and Pair Distribution Function in their application to environmental mineralogy. The subject is a hot topic and is very well presented, but a doubt naturally arises on its

place in a volume devoted to *crystallography*. The description of the structures would have benefited by the presence of some figures: only *one* structure is shown, at the very end of the chapter. Regrettably, we read on page 192 about the perfect sphalerite “lattice”: perhaps too much dealing with disorder is the reason for forgetting the fundamental difference between a lattice and a structure?

The fifth and last chapter (forty-two pages) presents aperiodic mineral structures and is authored by two of the world specialists in the field: Luca Bindi and Gervais Chapuis. After a much enjoyable historical perspective (hint to the reader: there are treasures hidden in the old literature! As Frank Henry Westheimer said, a couple of months in the laboratory can frequently save a couple of hours in the library...), the superspace approach needed to describe and interpret aperiodic crystals is introduced not only to explain their diffraction pattern, as usually done, but also to solve the problem in the indexing of faces, which with only three indices seem to contradict the law of rational indices. Symmetry in superspace (3+D space) is treated informally, in an intuitive way (for a formal and detailed approach there is plenty of literature), to leave enough space to the description and discussion of naturally occurring aperiodic crystals, including quasi-crystals.

In conclusion, this volume has its strong points in the clear, end-user friendly presentation of the topics, but is clearly skewed. It targets the nano- and disordered world (powder XRD, PDF, electron diffraction, with no single-crystal at all), goes in the superspace and confines three-dimensional ordered mineral structures in a chapter which is very extensive and well written but also a copy-and-paste of material appeared elsewhere. The reader has much to learn from this book, provided he/she is aware of the mentioned mistakes in the terminology and nomenclature. The content however covers only part of what the general title would suggest, although certainly on the “cutting edge”, as would say the professionals of the scientific communication.

## References

- Armbruster, T. & Danisi, R.M. (2015): Highlights in Mineralogical Crystallography. Berlin: DeGruyter, XII, 201 p.
- Hoppe, R. (1979): Effective coordination numbers (ECoN) and mean fictive ionic radii (MEFIR). *Z. Kristallogr.*, **150**, 23–52.
- Krivovichev, S.V. (2017): Structure description, interpretation and classification in mineralogical crystallography. *Crystallogr. Rev.*, **23**, 2–71.
- Nespolo, M. (2016): Charge Distribution as a tool to investigate structural details. IV. A new route to heteroligand polyhedra. *Acta Crystallogr.*, **B72**, 51–66.
- Takéuchi, Y. (1997): Tropochemical cell-twinning. A structure building mechanism in crystalline solids, Tokyo: Terra Scientific Publishing Company.