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6

Topological Crystallography

With a View Towards Discrete Geometric Analysis

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Volume 6

The history of science, from its very beginnings, is replete with great achievements facilitated by innovative mathematical thinking. Unfortunately, it is increasingly common for mathematics to be only loosely linked to the science, by an online device called Supplementary Material. This practice is especially common in biology, the heroic science our age, but it also is present in other fields.

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In future we therefore will strive to publish manuscripts that emphasize the dual roles of science and mathematics and which achieve the goal of scientific exposition that invites mathematical interest and vice versa.

Larry Sirovich
Editor-in-Chief

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Topological Crystallography

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Preface

The Russian mathematician P.L. Chebyshev (1815–1897) once said in a general context that the collaboration of theory and practice brings out the most beneficial results in the sciences. N.I. Lobachevskii, one of the discoverers of non-Euclidean geometry, also said, “There is no area of mathematics, however abstract, which may not someday be applied to phenomena of the real world”. Their statements pertain to what this work intends to convey to the reader; that is, the author wishes primarily to provide the reader with mathematical insight into modern crystallography, a typical practical science that originated in classifying the observed shapes of crystals. However, the tools we shall employ are not adopted from the traditional theory of crystallographic groups, but are rather from *algebraic topology*, a field in pure mathematics cultivated during the first half of the last century. More specifically, the elementary theory of covering spaces and homology is effectively used in the study of 3D networks associated with crystals. This explains the reason why this book is entitled *Topological Crystallography*.

Further, we formulate a minimum principle for crystals in the framework of *discrete geometric analysis*, which provides us with the concept of *standard realizations*, a canonical way proposed by the author and his collaborator Motoko Kotani in 2000 to place a given crystal structure in space so as to produce the most symmetric microscopic shape. In spite of its purely mathematical nature (thus having nothing to do with physical and chemical aspects of crystals), this concept, combined with homology theory, turns out to fit with a systematic design and enumeration of crystal structures, an area of considerable scientific interest for many years. Incidentally, crystallographers proposed a similar concept in their recent studies to determine the ideal symmetry of a crystal net and to analyze its topological structure.

The objects in topological crystallography are not necessarily restricted to structures of atomic scale, visible only through special devices. Ornamental patterns having crystallographic symmetry in art, nature, and architectures also fall within the scope of this book. Indeed, many interesting *forms* (*katachi* in Japanese) that are potentially useful for artistic designs in various areas can be generated from standard realizations.

Meanwhile, standard realizations show up in the asymptotic behaviors of random walks on *topological crystals*, the abstraction of crystal structures, and are closely related to a discrete analogue of *Abel–Jacobi maps* in algebraic geometry. These remarkable aspects of standard realizations, which are discussed in the final part of this book, indicate that topological crystallography is neither an outdated nor an isolated field in mathematics; it vigorously interacts with other areas in pure mathematics which have been intensively developed in the last decade. Thus this book, though devoted to a single application of mathematics, takes the reader to various mathematical fields.

The main target of this book is, naturally enough, both mathematicians (including graduate and even undergraduate students) and a wide circle of practical scientists (especially crystallographers and design scientists in art and architecture as well) who want to know how ideas and theories developed in pure mathematics are applied to a practical problem. This broad spectrum of readership will justify the style of our exposition in which basic material in mathematics occupies the first half of the book.

This work has grown out of the lecture notes that I prepared for my lectures at Meiji University during the academic year 2011–2012. I am grateful to Davide M. Proserpio, Jean-Guillaume Eon, and Michael O'Keeffe for fruitful discussions and for providing me with relevant references in chemical crystallography. I also thank Hisashi Naito and my daughter Kayo for producing the beautiful CG images of several hypothetical crystals. This work could not have been done without the friendly help and advice of several people, especially Polly Wee Sy and Tadao Oda. I take great pleasure in thanking them.

Kawasaki, Japan Toshikazu Sunada

Contents

List of Symbols

$\mathbb{Z}$	Additive group of integers
$\mathbb{Q}$	Set of rational numbers
$\mathbb{R}$	Set of real numbers
$\mathbb{Z}^n$	Additive group of n-ple integers
$\mathbb{R}^n$	n-Dimensional Euclidean space
$\mathbb{Z}_n (= \mathbb{Z}/n\mathbb{Z})$	Additive group of integers modulo n
$\|A\|$	Number of elements in a finite set A
$A \times B$	Cartesian product of sets A and B
$A \backslash B$ or $A - B$	Difference of A and B
$f : A \longrightarrow B$	A map of A into B
$f(C)$	Image of C $(\subset A)$ by f
Image f	Image of a map f
$f^{-1}(D)$	Inverse image of D $(\subset B)$ by f
$f\|C$	Restriction of a map $f : A \longrightarrow B$ to a subset C of A
$f \circ g$	Composition of $g : A \longrightarrow B$ and $f : B \longrightarrow C$
I	Identity map
$\dim W$	Dimension of a vector space W
$\operatorname{rank} A$	Rank of an abelian group A
$W_1 \oplus W_2$	Direct sum of abelian groups (or vector spaces) W_1 and W_2
$W_1 + W_2$	$\{w_1 + w_2 \mid w_1 \in W_1,\ w_2 \in W_2\}$
$\langle \mathbf{a}, \mathbf{b} \rangle$	Inner product of vectors $\mathbf{a}, \mathbf{b}$
$\\|\mathbf{a}\\| = \langle \mathbf{a}, \mathbf{a} \rangle^{1/2}$	Norm of a vector $\mathbf{a}$
Ker T	Kernel of a homomorphism T
$W^{\perp}$	Orthogonal complement of a subspace W
$M(m, n)$	Space of matrices of size (m, n)

I_n (or I)	Identity matrix of size n
$\det A$	Determinant of a square matrix A
$\mathrm{tr} A$	Trace of a square matrix A
${}^tA$	Transpose of a matrix A
B_n	n-Bouquet graph
K_n	Complete graph with n vertices
D_d	Graph with two vertices joined by $d+1$ parallel edges
$\deg x$	Degree of a vertex x
$\mathrm{Aut}(X)$	Automorphism group of a graph X
$C_1(X,\mathbb{Z})$	Group of 1-chains on a graph X with coefficients in $\mathbb{Z}$
$H_1(X,\mathbb{Z})$	1-st Homology group of a graph X with coefficients in $\mathbb{Z}$
$C_1(X,\mathbb{R})$	Group of 1-chains on a graph X with coefficients in $\mathbb{R}$
$H_1(X,\mathbb{R})$	1-st Homology group of a graph X with coefficients in $\mathbb{R}$
$b_1(X)$	Betti number of X
$\chi(X)$	Euler number of X
$\langle c \rangle$	1-Chain represented by a path c
$[c]$	Homotopy class of a closed path c
$\pi_1(X,x_0)$	Fundamental group of X with base point x_0
X_0^{uni}	Universal covering graph over a graph X_0
X_0^{ab}	Maximal abelian covering graph over a graph X_0
$E(\Phi,\rho)$	Normalized energy of a periodic realization (Φ,ρ)
Φ^{ab}	Normalized standard realization of X_0^{ab}
$p(n,x,y)$	n-Step transition probability
$\kappa(X_0)$	Tree number of a graph X_0
$[G,G]$	Commutator subgroup of a group G
$G_1 \times G_2$	Group product of two groups G_1 and G_2
$\mathbb{S}_n$	Symmetry group (group of permutations) of $\{1,2,\ldots,n\}$
$GL_n(\mathbb{R})$	General linear group
$GL_n(\mathbb{Z})$	Group consisting of integral square matrices A with $\det A = \pm 1$
$O(n)$	Orthogonal group
$SO(n)$	Special orthogonal group (rotation group)

Chapter 1
Introduction

> Mathematics allows us to understand the true nature of things by liberating us from the spell of the real world.

Applications of mathematics to crystallography have a long history. The theory of *crystallographic groups* (*space groups* in jargon) is a traditional field dating back to the first half of the nineteenth century, which, needless to say, has been playing a significant role in the classification of crystals in view of the symmetry.[1] Graph theory is another powerful area for the obvious reason that it is used to study the microscopic structure of a crystal[2] (and any molecule) as a 3D (three-dimensional) *network*,[3] in which each atom (or each cluster of atoms) is represented by a vertex of the net, and each edge of the net represents a *bond* (or a polymeric ligand) in the crystal structure.

A mathematical discipline that looks unconventional at first sight, but turns out to be an effective tool when applied to crystallography is *algebraic topology*, a field in geometry which studies structures of topological spaces by assigning algebraic data to topological spaces in order to translate topological problems into algebraic ones that hopefully will be more accessible [45]. This is by no means surprising because a graph is identified with a *cell complex* of one-dimension, and thus it is expected to be able to employ basic tools such as *covering spaces* and *homology*. Indeed, if a topologist is asked "What's the mathematical nature of crystal structures?", his

[1]To be precise, the notion of crystallographic groups has its origin in the study of *morphology* (the observed shapes) of crystals. In this sense, the link between mathematics and crystallography is ancient. See the beginning of Chap. 6.

[2]In this book, crystals mean solids composed of atoms arranged in an orderly repetitive array. In crystallography, more general materials such as quasicrystals are counted as crystals.

[3]Wells [109] initiated a systematic study of crystal structures as 3D networks. Applications of graph theory to chemistry could be traced back to 1864 when the Edinburgh chemist Crum Brown proposed representing chemical compounds by graphs.

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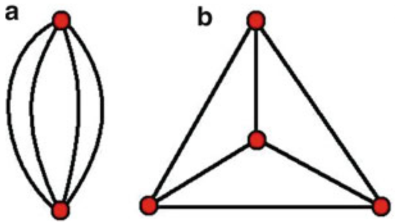

Fig. 1.1 "Seeds" of diamond, K_4 crystal, Lonsdaleite

immediate answer would be "topologically they are infinite-fold abelian covering graphs over finite graphs. The crystal nets (the networks in space associated with crystals) are their periodic realizations".

This bold answer is satisfactory enough, from the theoretical view at least, since among all abelian covering graphs over a given finite graph X_0, there is a *maximal* one from which we may construct, in a unified way, every abelian covering graphs over X_0. In fact, if one starts with a finite graph X_0 to obtain (hypothetical) 3D crystal structures,[4] then the main recipe in this construction is the selection of a subgroup H of $H_1(X_0,\mathbb{Z})$, the first integral homology group of X_0, such that the factor group $H_1(X_0,\mathbb{Z})/H$ is a free abelian group of rank-3, which is eventually going to be the *period lattice* when we realize the covering graph in space. A period lattice[5] here means a lattice group in $\mathbb{R}^3$ leaving a given crystal net invariant when it acts on the space $\mathbb{R}^3$ by translations (a more general definition is given in Sect. 7.1). In particular, the enumeration of topological structures of crystal nets reduces to that of finite graphs and subgroups of homology groups.

In a few cases, maximal abelian covering graphs themselves give 3D crystal structures. For instance, maximal abelian covering graphs over the graphs (A) and (B) in Fig. 1.1 yield the crystal structures of *Diamond*[6] and the hypothetical K_4 *crystal* (*diamond twin*),[7] respectively. On the other hand, *Lonsdaleite*[8] (Fig. 1.2[9]) is, as an abstract graph, a *non-maximal* abelian covering graph over the finite graph (C);

[4]By a *crystal structure* we mean an abstract graph associated with a crystal net.

[5]The notion of period lattices is a generalization of *Bravais lattices* in crystallography. Precisely speaking, a Bravais lattice is a representative of period lattices when classified by symmetry.

[6]Diamond is an allotrope of carbon which is formed and synthesized at high-pressure and high-temperature conditions, and is known to be less stable than graphite though the conversion rate from diamond to graphite is negligible at ambient conditions. Silicon and germanium adopt similar types of crystal structure.

[7]See Sect. 8.3 and Notes (IV) in Chap. 8 for the detailed account where we explain the reason why the K_4 crystal deserves to be called "diamond twin". The picture of the K_4 crystal is given in Fig. 1.4.

[8]This carbon allotrope, formed when meteorites containing *graphite* strike the earth, is named in honour of crystallographer Kathleen Lonsdale, also referred to as the *hexagonal diamond*.

[9]Source of the figure: WebElements (http://www.webelements.com/).

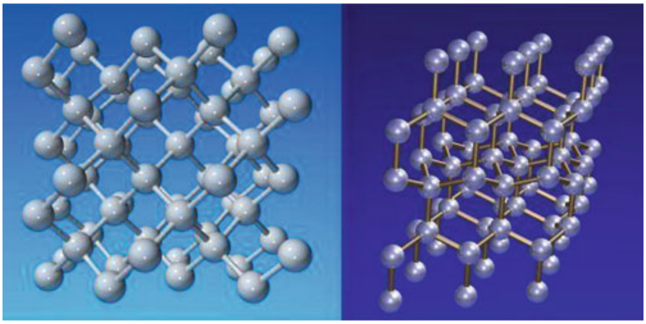

Fig. 1.2 Diamond and Lonsdaleite

indeed, the maximal abelian covering graph over (C) is five-dimensional. Therefore crystal structures of general dimension turn up even when we are handling three-dimensional crystals.

The simple answer above to the question about the mathematical nature of crystal nets is a sort of folklore in the community of mathematicians, and hence it is not attributed to anyone. It is no wonder, however, that Henri Poincaré (1854–1912), founder of algebraic topology, could have easily conceived this answer if he would have witnessed Max von Laue's discovery of crystal structures by the diffraction of X-rays, which was coincidentally accomplished in the last year of Poincaré's life.

Chemical crystallographers adopt the term "periodic graphs" for the underlying topology of crystal structures, based on the same reasoning as mathematicians that a crystal structure is a graph with a translational action which becomes a finite graph when factored out.[10] This difference of nomenclature[11] for the same objects makes crystallographers say "the rich world of periodic graphs has been largely neglected by mathematicians" [50]. The fact is that mathematicians have been interested in general covering spaces over cell complexes, not only of one-dimension but also of higher dimensions, and that our machinery in algebraic topology to tackle this important subject had been well developed long before. For all this, mathematicians' predisposition for liking general theories has hindered them from turning their eyes to crystal structures as illuminating examples of covering spaces.

The primary purpose of this book is to provide the reader with some fundamentals about "topological crystallography"[12] (or "topological methods in crystallography") in order to bridge the gap of knowledge between mathematicians and

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[10]They also use the term "minimal nets" for maximal abelian covering graphs [9] and the term "cycle spaces" for homology groups [42]. See Notes (V) in Chap. 8.

[11]Even for the description of crystallographic groups there are three main systems of notations; one used in mathematics, and other two (the Schoenflies system and International system) used by chemists and crystallographers.

[12]In chemistry, the term "topological crystal(lography)" is used sometimes in a different context.

crystallographers.[13] Thus no knowledge of algebraic topology and crystallography is presupposed. What the reader needs to be familiar with is basic material in undergraduate mathematics such as *sets, maps, matrices,vector spaces* (*with inner products*) and an elementary part of group theory (*abelian groups, homomorphism, factor groups*, etc.). Some of these prerequisites are briefly explained in the appendix for the convenience of the reader who is not knowledgeable about modern mathematics.

Moreover, this book is designed, for the most part, to be as self-contained as possible, taking into consideration as the reader practical scientists and undergraduate students with a modest background in mathematics. To accomplish this, we divide the book into three parts. Based on the fundamental material mentioned above, Part I starts with a quick review of the notions of quotient sets (Chap. 2) and graphs (Chap. 3). These notions are fairly standard in pure mathematics, and indispensable in modern crystallography. Subsequently, we provide a comprehensive account of homology (Chap. 4) and covering maps of graphs (Chap. 5) from the combinatorial viewpoint. Since they are usually not treated as independent topics in the literature of algebraic topology and combinatorics, we find it worthwhile to include these chapters here. Furthermore, the notions introduced in Chap. 5 will be useful in a set-up for the analysis and geometry of "non-commutative crystals", a generalization of crystal structures [see [95] and Notes (IV) in Chap. 9].

The contents up to this point are preliminaries to topological crystallography. The heart of the matter begins with Part II. After skimming through the preceding chapters, and if necessary going through the terminology employed as well as our own usage of notations, the reader having mathematics at his/her fingertips may then start from Chap. 6 containing some details about abelian covering graphs.

In this book, the term "topological crystal" is adopted for an infinite-fold abelian covering graph over a finite graph.[14] The reason is to emphasize its abstract nature and at the same time to keep the word "crystal" in order to make it clear that we are addressing the problem of crystals, not the problem of general graphs. In any case, topological crystals are purely mathematical objects "living in the logical world and not in real space", in the sense that they are constructed on the basis of pure reflection.[15]

The issue on how to place (realize) them "canonically" in space is discussed at length in Chap. 7, where we give a down-to-earth account, together with an algorithm (in a loose sense[16]) and many examples, of the mathematical construction

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[13]See the book [44] by J-G. Eon, W.E. Klee, B. Souvignier and J.S. Rutherford as a reference in crystallography.

[14]In [58], we have used the term "crystal lattice" instead.

[15]This is the so-called *Platonic view*; that is, we mathematicians insist that mathematical entities are abstract in not being spatiotemporally located, and hence lie outside of the real world.

[16]Algorithm means a step-by-step procedure involving a precise set of instructions for what to do next. With access to a computer and with some work in computer graphics based on our algorithm, 3D crystal structures may be displayed on a screen.

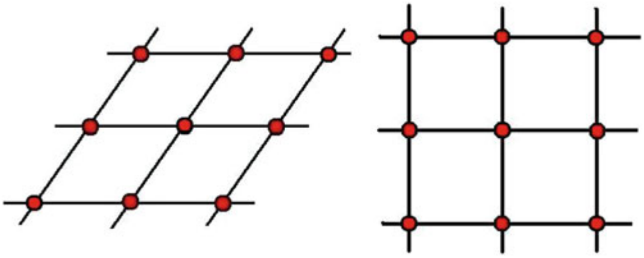

Fig. 1.3 A harmonic realization and the standard realization

stated in Kotani and Sunada [58]. The *standard realization*[17] spelled out here is most symmetric among all realizations (hence deserves to be described as “standard”), and is characterized uniquely by a *minimal principle* for the potential energy (per unit cell) when we look at a realization as a simple system of harmonic oscillators. This may remind the reader of the classical *isoperimetric inequality* characterizing the *round circle*, the most symmetric closed curve.[18]

One remark is in order here. Crystallographers also sought independently canonical ways to place periodic graphs and thus proposed several notions:

1. *Archetype embedding* [42]. This turns out to be the same as the standard realization of the maximal abelian covering graph.
2. *Equilibrium placement* [30]. This notion, inspired by Tutte [102, 103] and suggested by Klein [55], coincides with the *harmonic realization* introduced in [58] as a special case of *harmonic maps* [39, 69] [see Notes (IV) in Chap. 7]. Roughly speaking, harmonic realizations (equilibrium placements) are characterized as minimizers[19] of the energy functional *when a period lattice is fixed.*[20] On the other hand, standard realizations are minimizers *without any constraint on period lattices* (except for the one on the volume of unit cells). Therefore standard realizations are special harmonic realizations (Fig. 1.3 illustrates the difference between a general harmonic realization and the standard realization in the case of the quadrangle lattice). Based on the notion of equilibrium placement, Delgado-Friedrichs constructed a poweful algorithm (*SYSTRE*[21]) for the *barycentric drawing*, a special equilibrium placement (see [32]), which seems to coincide with the standard realization as far as several examples are examined (at least in the two-dimensional case).

[17] In [96], I used the term “canonical placement”.

[18] For a closed curve in the plane, if its perimeter is L and the area that it encloses is A, then $4\pi A \leq L^2$, where equality holds if and only if the curve is a circle.

[19] A *minimizer* of a given function (or functional) is a point (or function) at which the minimum value is attained.

[20] Fixing a period lattice is equivalent to imposing a periodic boundary condition.

[21] The program is available at http://www.gavrog.org/.

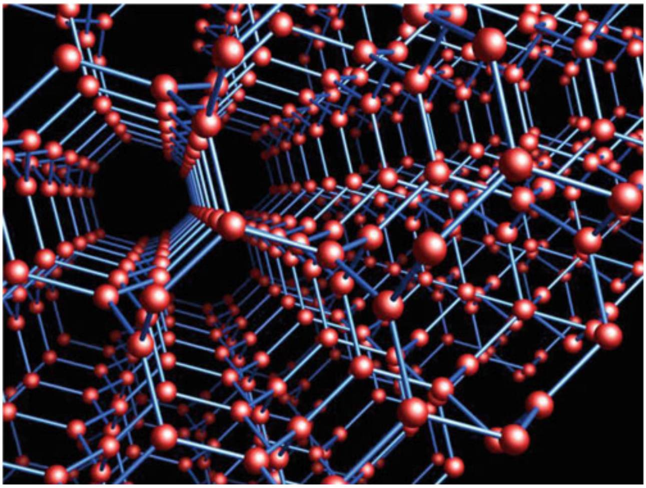

Fig. 1.4 CG image of the K_4 crystal (created by Kayo Sunada)

3. *Archetypical representation* [43]. This is an appropriate orthogonal projection of the archetype embeddings, and turns out to be identical to the standard realization (see Chap. 8).

Admittedly the nature of standard realizations is purely mathematical, and has almost nothing to do with the physical and chemical aspects of real crystals. Thus one can say that the nets obtained by standard realizations are merely toy models of hypothetical crystal,[22] i.e., not necessarily in actual existence. Nevertheless, as will be observed in Chap. 8, the nets corresponding to several typical real crystals turn out to be canonically placed in our sense. Diamond and Lonsdaleite are such examples. The nets obtained from the *face-centered cubic lattice* and the *body-centered cubic lattice* are also standard realizations. Incidentally, the hypothetical K_4 crystal mentioned above is constructed by means of a standard realization (Fig. 1.4).

The nets of real crystals are usually different from the standard realization because the mechanism of crystallization is much more complicated than the one explained by the harmonic-oscillator model for a crystal. Even in this case, however, the standard realization offers, in the light of its uniqueness, a basis for comparison with which one may talk quantitatively about how much the net is distorted (Sect. 7.5).

Apart from crystallography handling forms of Angstrom scale, the concept of standard realization is of some interest from the view of beautiful "ornamental patterns" that are visible to the naked eye, both in nature and art, such as the

[22]Once we find a hypothetical crystal, a systematic prediction of its physical properties for appropriate atoms can be carried out by *first principles calculations* used in chemistry. The prediction appealing to the computer power encourages (or discourages) material scientists to synthesize the hypothetical crystals [26].

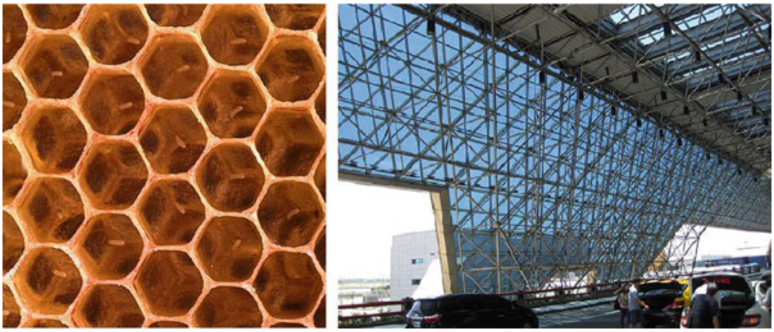

Fig. 1.5 Patterns in nature and architecture

honeycomb pattern built by beehives which is used in countless artistic structures. The honeycomb is actually the standard realization of the *hexagonal lattice*,[23] a two-dimensional topological crystal described as the maximal abelian covering graph over the graph with two vertices joined by three parallel edges; thus the net of diamond crystal is regarded as the three-dimensional analogue of the honeycomb; see Sect. 8.3.

What is more, the beauty of shapes is somehow bound up with the mechanical functions of architectural structures e.g., as beehives instinctively know that their honeycomb is the best structure to reach minimal weight and minimal material cost. The picture on the right side in Fig. 1.5 is a light weight rigid structure in architecture (due to Alexander Graham Bell and Buckminster Fuller), which turns out to tie up with the net associated with the face-centered cubic lattice, an example of standard realizations as mentioned above; see Sect. 8.3 (III).

Let us return to the structure of the book. Part III, mainly targeting mathematicians and graduate students, is concerned with two idiosyncratic topics closely related to standard realizations; more specifically, we deal with *random walks* on topological crystals, and a discrete analogue of classical algebraic geometry. I would like to emphasize that a remarkable relation between random walks and standard realizations, the subject in Chap. 9, is my starting point to develop topological crystallography. Chapter 10 introduces the notion of *discrete Abel–Jacobi map* which is relevant to the standard realizations of maximal abelian covering graphs. What we discuss in this final chapter is considered a ramification of algebraic graph theory and also of *tropical geometry*, a relatively new and thriving area.

Each chapter ends with a section entitled “Notes” wherein, except for historical remarks added for the pedagogical reason, we make liberal use of concepts in

[23]The usage of the term “lattice” for crystal structures may give rise to confusion because customarily a lattice means a discrete subgroup of $\mathbb{R}^d$ (or more generally a discrete subgroup of a Lie group). But we will follow the convention to use “lattice” for some crystal structures (see Remark in Sect. 2.2).

advanced mathematics. The overall purpose is to inform the reader, somewhat in a rambling style, how the subject discussed in the chapter is related to other fields of mathematics, say, the Ihara zeta function, a graph-theoretic analogue of class field theory, discrete Laplacians, and harmonic maps. Although not necessarily needed for what follows in Parts I and II, it offers the reader with a mathematical bent some additional insights into our subject and a underlying motive. Part III also has a similar nature, and may give a surprise to the reader. He or she will discover that a problem in one area leads us into a quite different area of mathematics.

In writing this book, I followed the conventional style of mathematical books. That is, in accordance with mathematics culture, I will give proofs to almost all claims that the reader might find difficult to verify by himself/herself (except for those in Notes). The reason for doing so is that I want to remind the reader of the significant function of proofs. Proofs in mathematics play the same role as verifications by experiments in other sciences.[24] In view of this, I strongly recommend the reader (even a practical scientist) to try to understand proofs.

[24] A "proof" is a logical procedure to derive what we anticipate to be true from what we have already known to be true.

Part I
Prerequisites for Modern Crystallography

Chapter 2
Quotient Objects

Crystallographers employ the concept of "quotient graph" in a systematic enumeration of crystal structures (see for instance [20, 41, 76, 86]). Behind this concept is the periodic nature of crystal structures with respect to parallel translations; that is, a quotient graph in crystallography is nothing but the quotient graph of a 3D network by the translational action of a lattice group; see the next chapter for details.

As a matter of fact the idea of "quotient" shows up in various fields of modern mathematics; say, *quotient vector spaces* in linear algebra, the *cut-and-paste technique* in topology, *coset spaces* and *factor groups* in group theory, to name several. If we identify graphs with one-dimensional cell complexes,[1] then a quotient graph is a special case of *quotient spaces* introduced in topology. Even if our discussion is confined to crystallography, the reader will come across many quotient objects.

Related to the idea of "quotient" is the word "well defined". This rather strange locution is used when we want to define a new object such as a map or an operation among quotient objects and we need to ensure the consistency of the definition. The issue of well-definedness is hardly avoided in modern mathematics. Beginners are expected to get used to it by verifying many examples appearing in our discussion.[2]

Hereafter the reader is assumed to know set-theoretic language and some basic notions in group theory. I recommend the reader to consult Appendices 1 and 2 for the meaning of the terminology used in this chapter.

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[1]A cell complex is a topological space obtained by gluing together certain basic building blocks called cells. Here an n-dimensional cell is a topological space that is homeomorphic to an n-dimensional closed ball.

[2]According to my experience, the issue of well-definedness is often a hindrance to students who are struggling to learn modern mathematics.

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2.1 Equivalence Relations

The meaning of "quotient" is roughly interpreted as follows. Suppose we are given an aggregation of objects (animals or plants for instance). We classify these objects according to certain properties, and form groups by gathering classified objects. Following this procedure, we give a name to each group (mammals, birds, reptiles, etc., for animals). Then the set of names is what we call the *quotient set*.

One can make this plain-language explanation rigorous by introducing the notion of equivalence relations as follows. Let A be a set with a *relation* $\sim$ among elements in A. More precisely, we are given a subset R of the cartesian product $A \times A$ with which the statement "$(x,y) \in R$" is read "x is related to y" and is written $x \sim y$. A relation $\sim$ satisfying the following three conditions is said to be an *equivalence relation*.

1. $x \sim x$ for every x.
2. If $x \sim y$, then $y \sim x$.
3. If $x \sim y$ and $y \sim z$, then $x \sim z$.

When $x \sim y$ for an equivalence relation $\sim$, we say that x and y are *equivalent* (what we have in mind is a statement like "x and y have the same property"). In essence, an equivalence relation is a generalization of equality "$=$" which, of course, satisfies the above conditions.

The equivalence relation yields a partition of A as follows. For $x \in A$, we denote by $E(x)$ the *equivalence class* of x; that is, the subset consisting of all elements equivalent to x. Then $x \in E(x)$, and either $E(x) \cap E(y) = \emptyset$ (empty set) or $E(x) = E(y)$, which implies that different equivalence classes do not overlap, and they cover the whole set A, thereby inducing a partition of A. Conversely, a partition of A yields an equivalence relation in a natural manner.

Now consider the set of equivalence classes for which we use the notation $A/\sim$, and call it the *quotient set* with respect to the relation $\sim$. Therefore each equivalence class, originally a subset of A, becomes a single element in the quotient set $A/\sim$. The *canonical projection* is the map $p : A \longrightarrow A/\sim$ that carries $x \in A$ into the equivalence class of x.

Useful later on in our discussion is the following observation. Let A and B be two sets with equivalence relations $\sim_A$ and $\sim_B$, respectively, and let $f : A \longrightarrow B$ be a map having the property that if $x \sim_A y$, then $f(x) \sim_B f(y)$. For the canonical projections $p_A : A \longrightarrow A/\sim_A$ and $p_B : B \longrightarrow B/\sim_B$, there is a map $F : A/\sim_A \longrightarrow B/\sim_B$ such that $F \circ p_A = p_B \circ f$. The following diagram, called a *commutative diagram*, will help the reader understand visually this equality of maps.