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Hisashi Naito

Trivalent Discrete Surfaces and Carbon Structures

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In memory of my wife Yumiko.

Preface

Topological crystallography, which was pioneered by Motoko Kotani and Toshikazu Sunada in 2000, describes crystal structures using graph theory and variational principles. One of the conventional tools describing crystal structures is space groups, which denote the symmetry of placements of atoms. But space groups do not consider the atomic bonds of crystals. Since crystal structure includes placements of atoms and chemical bonds between atoms, graph theory is a natural tool to describe them. On the other hand, one of the important notions to describe physical phenomena is the principle of least action, which corresponds to the variational principle in mathematics.

Although the description of crystal structures using space groups is not directly related to the least action principle, topological crystallography provides a relationship between the symmetry of crystal structures and the variational principle. Precisely, for a given graph structure which describes a crystal, we define the energy of realizations of the graph, i.e., placements of vertices of the graph in a Euclidean space of suitable dimension, and obtain a nice structure as a minimizer of the energy. Moreover, such structures give us the most symmetric among all placements of the graph, which is proved by using the random walk theory on graphs.

On the other hand, we can regard some molecular structures, for example, fullerenes and carbon nanotubes, as surfaces, especially as discrete surfaces. Recently, sp^2-carbon structures (including fullerenes and nanotubes) have received much attention in science and technology, since they have rich π-electrons and hence rich physical properties. From a mathematical viewpoint, sp^2-carbon structures can be regarded as trivalent graphs in $\mathbb{R}^3$, and hence trivalent *discrete surfaces*. There are many discrete surface theories in mathematics. For example, the theory of triangular surfaces is useful for computer graphics. But this is based on discretizations or discrete analogues of continuous or smooth objects. In the case of the theory of triangular surfaces, it is a discretization of smooth real objects. In other words, conventional discrete surface theories are "from continuous to discrete". In contrast, discrete surfaces, which describe crystal/molecular structures, are essentially discrete. Even in the case of trivalent discrete surfaces, it is not easy to define the curvatures of them. In this monograph, we also discuss a theory of trivalent discrete surfaces modeled on

crystal/molecule structures in $\mathbb{R}^3$, and subdivisions/convergence of them. The aim of subdivision and convergence theory is to find an underlying continuous object in crystals/molecules. It is difficult to calculate the physical properties of a crystal structure with a huge number of atoms using current computer resources; however, it is possible to treat such systems by calculating underlying continuous objects. By considering the above, our discrete surface theory is "from discrete to continuous".

I would like to thank Prof. Motoko Kotani for encouraging me to write this monograph, and Prof. Toshikazu Sunada for leading me to the study of discrete geometric analysis. I would also like to thank Profs. Tatsuya Tate, Makoto Tagami, Yoshiyuki Kawazoe, and Hiroyuki Isobe, Dr. Toshiaki Omori, Dr. Shintaro Akamine, and members of the research project "Discrete Geometric Analysis for Material Design" for helpful discussions and comments on my research. I am grateful to Dr. Tomoya Naito for his valuable comments and suggestions. Lastly, I would like to thank the members of the Japanese girls group "Nogizaka46" for encouraging my research.

Enjoy a discrete world!

Nagoya, Japan Hisashi Naito
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Chapter 1
Overview of This Monograph

Let us start with a question here. Which figure in Fig. 1.1 is the most symmetric?

Obviously, figure (c) in Fig. 1.1 has less symmetry than (a) and (b); however, it is difficult to compare symmetries of (a) and (b).

One of the basic tools for describing symmetries of crystal structures is space groups, which describe symmetry of atoms (vertices/points) in a crystal structure. For example, the symmetry of a regular hexagonal tiling of $\mathbb{R}^2$ is described by the group $P6m$, and the space group of the symmetry of a regular three-colored hexagonal tiling (see Fig. 1.2b) is $P3m1$. Similarly, the group $P6m$ describes the symmetry of a regular hexagonal lattice. The groups describing the symmetry of (a) and (b) of Fig. 1.1 are $P4mm$ and $P6m$, respectively, and one is never included in the other.

Topological crystallography, which was pionnered by Kotani and Sunada [28–30, 54], describes symmetries of both of vertices and of edges (atomic bonds of crystal structure). Why does nature select (b) among (a)–(c) in Fig. 1.3? Note that these lattices are created by the same graph. Topological crystallography answers this question. In mathematics, a structure consisting of vertices and edges (connectivity of vertices) is called a graph, and graph theory is one of the basic tools of topological crystallography (Chap. 2). However, graphs describe only vertices and their connectivities, as in Fig. 2.2; placements of vertices and edges in $\mathbb{R}^n$ are not defined in the notion of graphs. Therefore, we should define placements of a given graph structure, which describes crystal structure, and should consider how to define *nice placement* of the graph. By defining the energy of placements of a graph, we may find a nice placement, which is called a *standard realization*, by using variational principles. A standard realization gives us one of the most symmetric objects among all placements of the graph (Chap. 3). In the first few sections, we discuss topological crystallography including graph theory and geometry. The most important reference of this part is Sunada's lecture note [53]. The author discusses an introduction to topological crystallography along with it.

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