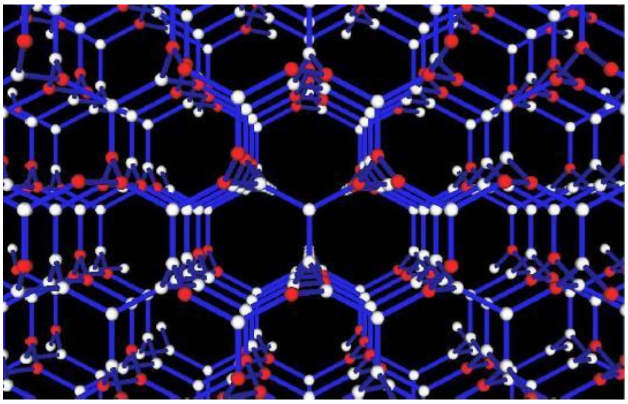
MIMS Technical Report No.00032 (201105081)

Topological Crystallography

—In view of Discrete Geometric Analysis—



Toshikazu Sunada

PREFACE

Russian mathematician P. L. Chebyshev (1815-1897) once said in a general context that the agreement of theory and practice brings most beneficial results in sciences. His words pertain to what this monograph intends to convey to the reader. That is, the author wishes primarily to provide the reader with a mathematical insight into modern crystallography, a typical practical science that originated in the classification of the observed shapes of crystals. However the tools we shall employ are not adopted from the traditional theory of crystallographic groups, but from *algebraic topology*, a field in pure mathematics cultivated during the last century. More specifically the theory of covering spaces and homology theory are effectively used in the discussion on the 3D networks associated with crystals. This explains the reason why this monograph is entitled *Topological Crystallography*. Further we formulate a minimum principle for crystals in the framework of *discrete geometric analysis*, which, in spite of its pure-mathematical nature, turns out to fit with a systematic enumeration of crystal structures, an area of considerable scientific interest for many years.

The objects that topological crystallography concerns are not necessarily restricted to crystals. Ornamental patterns having crystallographic symmetry in art, nature and architectures are the objects falling within the scope of this monograph. Indeed, many interesting *forms* (*Katachi* in Japanese) which are potentially useful for artistic designs in various areas are generated from *canonical placements* characterized by the minimum principle. Therefore, the main target of this monograph 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 monograph has developed out of the note that I prepared for my lectures at Meiji University during the academic year 2011-12. My thanks are due to Davide M. Proserpio who provided 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. I have great pleasure in thanking her.

Toshikazu Sunada

Contents

Bibliography

[1] I. V. Artamkin, *Discrete Torelli theorem*, Sbornik: Mathematics **197** (2006), 1109-1120.

[2] R. Bacher, P. De La Harpe, and T. Nagnibeda, *The lattice of integral flows and the lattice of integral cuts on a finite graph*, Bull. Soc. Math. France, **125** (1997), 167–198.

[3] M. Baker and S. Norine, *Riemann-Roch and Abel-Jacobi theory on a finite graph*, Adv. in Math., **215** (2007), 766–788.

[4] H. Bass, *The Ihara-Selberg zeta function of a tree lattice*, International. J. Math., **3** (1992), 717–797.

[5] N. L. Biggs, *Algebraic Graph Theory*, Cambridge University Press, 1993.

[6] N. L. Biggs, *Algebraic potential theory on graphs*, Bull. London Math. Soc., **29** (1997), 641–682.

[7] V. Blatov, *Search for isotypism in crystal structures by means of the graph theory*, Acta Cryst. **A56** (2000), 178–188.

[8] B. Bollobas, *Modern Graph Theory*, Springer, 1998.

[9] L. Caporaso and F. Viviani, *Torelli theorem for graphs and tropical curves*, Duke Math. J., **153** (2010), 129–171.

[10] S. J. Chung, T. Hahn, and W. E. Klee, *Nomenclature and generation of three-periodic nets: the vector method*, Acta. Cryst., **A40** (1984), 42–50.

[11] L. S. Charlap, *Bieberbach Groups and Flat Manifolds* Springer-Verlag, 1986.

[12] J. H. Conway, H. Burgiel, C. Goodman-Strauss, *The Symmetries of Things*, A K Peters Ltd, 2008.

[13] , H. S. M. Coxeter, *Regular complex Polytopes*, Cambridge University Press, 1974.

[14] , P. Cromwell, *Polyhedra*, Cambridge University Press, 1999.

[15] S. Curtarolo, D. Morgan, K. Persson, J. Rodgers, and G. Ceder, *Predicting crystal structures with data mining of quantum calculations* Phys. Rev. Lett., **91** (2003), 135503.

[16] O. Delgado-Friedrichs and M. O'Keeffe, *Identification of and symmetry computation for crystal nets*, Acta Cryst., **A59** (2003), 351–360 .

[17] O. Delgado-Friedrichs, M. O'Keeffe and O. M. Yaghin, *Three-periodic nets and tilings: regular and quasiregular nets*, Acta Cryst., **A59** (2003), 22–27.

[18] O. Delgado-Friedrichs, *Barycentric drawings of periodic graphs*, LNCS **2912** (2004), 178–189.

[19] W. Ebeling, *Lattices and Codes*, Vieweg, 1994.

[20] J. Eells and J. H. Sampson, *Harmonic mappings of Riemannian manifolds*, Amer. J. Math., **86** (1964) 109–160.

[21] O. Friedrichs, A. Dress, D. Huson, J. Klinowski and A. Mackay, *Systematic enumeration of crystalline networks*, Nature **400** (1999), 644–647.

[22] M. Greenberg, *Lectures on Algebraic Topology*, Benjamin, 1971.

[23] M. Gromov. *Metric Structures for Riemannian and Non-Riemannian Spaces*, Birkhäuser, 1999.

[24] S. T. Hyde, M. O'Keeffe, and D. M. Proserpio, *A short history of an elusive yet ubiquitous structure in chemistry, materials, and mathematics*, Angew. Chem. Int. Ed., 2008, **47**, 2–7

[25] Y. Ihara, *On discrete subgroups of the two by two projective linear group over p-adic fields*, J. Math. Soc. Japan, **18** (1966), 219-235.

[26] A. Katsuda and T. Sunada, *Closed orbits in homology clasees*, Publ. Math. IHES. **71** (1990), 5–32.

[27] E. Koch and W. Fischer, *Sphere packings with three contacts per sphere and the problem of the least dense sphere packing*, Z. Kristallogr., **210** (1995), 407–414.

[28] M. Kotani and T. Sunada, *Zeta functions of finite graphs*, J. Math. Sci. Univ. Tokyo **7** (2000), 7–25.

[29] M. Kotani and T. Sunada, *Standard realizations of crystal lattices via harmonic maps*, Trans. Amer. Math. Soc., **353** (2000), 1–20.

[30] M. Kotani and T. Sunada, *Jacobian tori associated with a finite graph and its abelian covering graphs*, Advances in Apply. Math., **24** (2000), 89-110.

[31] M. Kotani and T. Sunada, *Albanese maps and off diagonal long time asymptotics for the heat kernel*, Comm. Math. Phys., **209** (2000), 633–670.

[32] M. Kotani and T. Sunada, *Spectral geometry of crystal lattices*, Contemporary Math., **338** (2003), 271–305.

[33] M. Kotani and T. Sunada, *Large deviation and the tangent cone at infinity of a crystal lattice*, Math. Z., **254** (2006), 837–870.

[34] J. Milnor, *Morse Theory*, Princeton University Press, 1969.

[35] T. Nagano and B. Smith, *Minimal varieties and harmonic maps in tori*, Comm. Math. Helv., **50** (1975), 249–265.

[36] T. Nagnibeda, *The Jacobian of a finite graph*, Contemporary Math., **206** (1997), 149–151.

[37] P. Newman, G. Stoy, and E. Thompson, *Groups and Geometry*, Oxford University Press, 1994.

[38] A. Oganov (Ed.), *Modern Methods of Crystal Structure Prediction*, Wiley-VCH, 2010.

[39] T. Nagano and B. Smith, *Minimal varieties and harmonic maps in tori*, Comm. Math. Helv., **50** (1975), 249–265.

[40] M. O'Keeffe, *N-dimensional diamond, sodalite and rare sphere packings*, Acta Cryst., **A47** (1991), 748–753.

[41] E. Peresypkina and V. Blatov, *Molecular coordination numbers in crystal structures of organic compounds*, Acta Crystallogr., **B56** (2000), 501–511.

[42] H. Resnikoff and R. Wells, Jr., *Wavelet Analysis*, Springer, 1998.

[43] L. Scott, *A Primer on Ice*, in preparation.

[44] J. P. Serre, *Trees*, Springer-Verlag, 1980.

[45] M. Shubin and T. Sunada, *Mathematical theory of lattice vibrations and specific heat*, Pure and Appl. Math. Quaterly, **2** (2006), 745-777.

[46] R. Strong and C. J. Packard. *Systematic prediction of crystal structures: An application to* sp^3*-hybridized carbon polymorphs*, Phy. Review B, **70** (2004), 045101.

[47] T. Sunada, *Riemannian coverings and isospectral manifolds*, Ann. of Math., **121** (1985), 169–186.

[48] T. Sunada, *L-functions in geometry and some applications*, Proc. Taniguchi Symp. 1985, "Curvature and Topology of Riemannian Manifolds", Springer Lect. Note in Math. **1201** (1986), 266-284.

[49] T. Sunada, *Fundamental groups and Laplacians*, Proc. Taniguchi Symp. "Geometry and Analysis on Manifolds", 1987, Springer Lect. Note in Math. **1339** (1988), 248-277.

[50] T. Sunada, *Why do Diamonds Look so Beautiful ?*, Springer, Tokyo, 2006 (in Japanese).

[51] T. Sunada, *Crystals that nature might miss creating*, Notices Amer. Math. Soc., **55** (2008), 208–215.

[52] T. Sunada, *Discrete geometric analysis*, Proceedings of Symposia in Pure Mathematics, (ed. by P. Exner, J. P. Keating, P. Kuchment, T. Sunada, A. Teplyaev), **77** (2008), 51–86.

[53] J. H. van Lint and R. M. Wilson, *A Course in Combinatorics*, Cambridge University Press, 1992.

[54] J. W. Vick. *Homology Theory*, Second Edition, Springer-Verlag, 1994.

[55] A. F. Wells, *Three Dimensional Nets and Polyhedra*, Wiley (1977).

[56] H. Weyl, *Symmetry*, Princeton University Press, 1983.

[57] J. A. Wolf, *Spaces of Constant Curvature*, McGRAW-HILL, 1967.

[58] E. A. Wood, *Crystals and Light –An Introduction to Optical Crystallography–*, Second Revised Edition, Dover, 1977.