01

Principles of the structural design of photonic quasicrystals

© A.E. Madison

HSE University, St. Petersburg, Russia
E-mail: alex_madison@mail.ru

Received April 18, 2024
Revised May 24, 2024
Accepted June 5, 2024

A theory of the structure of icosahedral quasicrystals is being developed based on the tiling theory and the concept of unit cells. An algorithm is proposed that includes filling several types of unit cells with atoms according to the local matching rules and filling the space with unit cells through inflations and deflations. The theory makes it possible to design the structures of icosahedral quasicrystals of all the three types within both groups of icosahedral symmetry, including the right-handed and left-handed enantiomorphic forms..

Keywords: photonic crystals, icosahedral quasicrystals, tiling, substitution rules.

DOI: 10.61011/TPL.2024.10.59686.19962

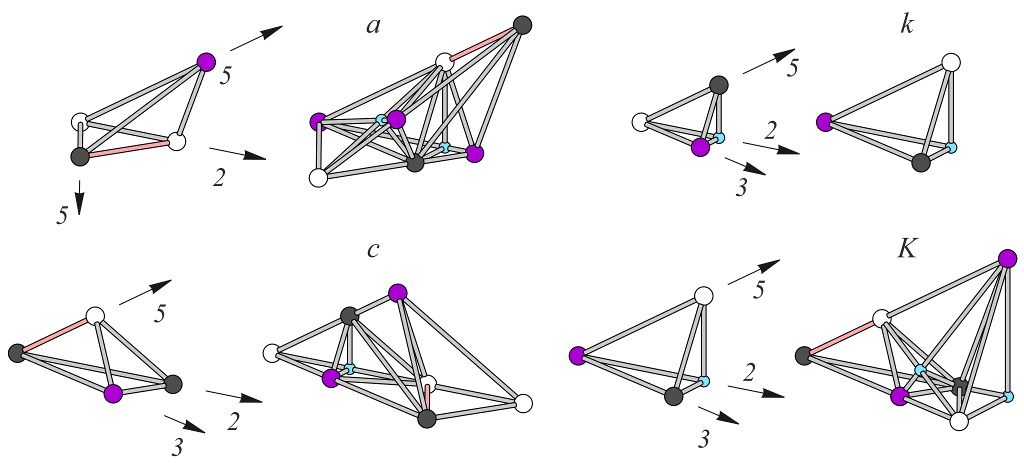
Aperiodic ordering opens up prospects for the production of new materials and structures with unusual properties. Extensive research efforts aimed at creating new types of quasicrystalline alloys, metamaterials, materials from non-atom building blocks, and aperiodic deterministic structures are currently underway [1,2]. Photonic quasicrystals [3–5] belong to a special class of structures with aperiodic order. The design of possible photonic crystal structures has long relied on analogies with periodic crystal lattices. Aperiodic photonic materials may offer fundamentally new possibilities for control and management of light fluxes, potentially even fulfilling the dream of an „invisibility cloak" [6]. Since the produced materials have no natural counterparts, the development of theoretical principles of targeted design of their structures becomes important [7]. The higher-dimensional approach [8,9] has limited applicability for designing photonic quasicrystal structures, which is why alternative techniques [10–12] become relevant.

We are developing a theory of the structure of icosahedral quasicrystals based on the tiling theory and the concept of unit cells [13–17]. The structural design of photonic quasicrystals involves two subproblems: filling the space with cells and filling the cells with atoms. An iterative inflation and deflation algorithm is used instead of translations to fill the space with cells, and copies of several types of unit cells should be used instead of a single one. Unit cells must satisfy local matching rules. The method of filling a cell with specific atoms should be defined uniquely by its type.

The following two tilings obtained by projection from 6D space and consistent with the concept of unit cells are known: the Socolar–Steinhardt tiling into four types of zonohedra [18] and the *ABCK* Danzer tiling into four types of tetrahedra [19]. They are characterized by different inflation factors, although Danzer himself has pointed out their complete equivalence in the sense of mutual local derivability [20]; i.e., polyhedra of one of them may be dissected into smaller parts, which may then be regrouped into polyhedra of the second tiling (see [21], p. 235). Thus, there should exist a certain tiling into smaller subunits from which both tilings may be constructed.

Three types of icosahedral quasicrystals (P, I, F) may be obtained by projecting six-dimensional counterparts of the primitive, body-centered and face-centered cubic lattices, respectively [22]. The Socolar–Steinhardt tiling is constructed on six basis vectors and corresponds to type P. The Danzer tiling is derived from the $D6$ root lattice and, consequently, should correspond to type F. The F-type polytope centering scheme is obtained by combining a primitive six-dimensional hypercubic lattice with several of its translations and includes types P (one original sublattice) and I (a combination of two sublattices) as subsets (see [9], p. 177). Therefore, there should exist three types of mutually consistent tilings that could form the basis for structural characterization of all three types of icosahedral quasicrystals.

The first one is the Socolar–Steinhardt tiling into golden zonohedra. The second one is the Danzer tiling [19], but, instead of the four Danzer tetrahedra (A, B, C, K), we use their copies reduced in size by a factor of τ (a, b, c, k), where τ is the golden ratio. The basis set of cells in the third tiling of interest to us is (a, c, k, K). It is formed by three Danzer tetrahedra A, C, K reduced in size by a factor of τ and one tetrahedron K of the original size. Note that the basis set of tetrahedra of the $ackK$ tiling is also derived from the $D6$ root lattice by projecting its Voronoi polyhedron [23]. An equivalent (up to inflation) tiling was mentioned by Danzer [19] in the section titled „Unsolved Problems." The primary issue was whether the two tetrahedral tilings mentioned above are in some sense isomorphic to each other and, if not, what is the fundamental difference between them. The problem has remained unsolved for several decades, and the second tetrahedral tiling mentioned by Danzer has remained virtually unexplored. The present paper fills this gap to a certain extent.



Substitution rules for the $ackK$ tiling. The edges of tetrahedra are oriented along the corresponding axes of symmetry of an icosahedron. Vertices of different types are colored differently: A (white), B (black), C (magenta), and F (blue). The inflation factor is τ. A color version of the figure is provided in the online version of the paper.

The substitution rules for the $ackK$ tiling are shown in the figure. Substitutions are characterized by the substitution matrix or the composition matrix transposed to it. In the latter case, one may use a formal matrix equation with the usual row-by-column multiplication rule:

$$\text{infl}\begin{pmatrix} a \\ c \\ k \\ K \end{pmatrix} = \begin{pmatrix} 0 & 2 & 3 & 3 \\ 1 & 2 & 2 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 2 & 3 \end{pmatrix} \begin{pmatrix} a \\ c \\ k \\ K \end{pmatrix}.$$

There are four types of vertices in the tiling. We use Roman letters to denote vertices (A, B, C, F) and italic letters for tetrahedra (as a reminder, capital letters A, B, C, K are traditionally used to denote Danzer tetrahedra, and their copies reduced in size by a factor of τ are designated here with lowercase letters a, b, c, k). Vertices A, B, C in the resulting tilings correspond to three types of nodes with local icosahedral symmetry. They cyclically replace each other after each iteration: C→B→A→C. Therefore, the inflation factor is equal to golden ratio τ, and the self-similarity factor of the packing as a whole is τ^3. There are two types of edges [AB] of the same length that differ in the local matching rules. Edges of the second type are highlighted in light red in the figure (a color version is provided online) to emphasize the analogy with the corresponding edges of the zonohedral tiling [13–17].

There is an exact mutual correspondence between the $ackK$ tiling and the Socolar−Steinhardt tiling. Nodes C were lacking initially in the zonohedral tiling [18]. We added them [13]. If one also adds nodes F to the centers of the triacontahedron faces and to equivalent positions, all nodes in both tilings will match completely. Zonohedra (prolate rhombohedron (GR), rhombic dodecahedron (RD), rhombic icosahedron (RI), and rhombic triacontahedron (RT)) are composed of tetrahedra in accordance with equation

$$\begin{pmatrix} GR \\ RD \\ RI \\ RT \end{pmatrix} = \begin{pmatrix} 0 & 6 & 12 & 0 \\ 8 & 12 & 4 & 4 \\ 10 & 10 & 0 & 40 \\ 0 & 0 & 0 & 120 \end{pmatrix} \begin{pmatrix} a \\ c \\ k \\ K \end{pmatrix}.$$

If nodes C in different types of zonohedra are regarded as different ones, zonohedra may be used as unit cells in the description of P-type quasicrystals.

If nodes C are added into zonohedra, the zonohedra are broken down into tetrahedra in the manner described above, and all tetrahedra of the same type are equivalent to each other, the packing corresponds to I-type quasicrystals. The tetrahedra of the resulting $ackK$ tiling may be used as unit cells. When decorating them with specific atoms, one needs to take into account the following possible non-equivalent positions: four types of nodes (three of which have local icosahedral symmetry), 10 positions on different edges, 12 positions on different faces, and four positions within each tetrahedron.

The $ackK$ tiling needs to be converted into the $abck$ Danzer tiling to obtain F-type icosahedral packing. This may be achieved by presenting all tetrahedra K as the unions of two tetrahedra b and k (one additional node C then emerges on edge [CF] of each tetrahedron K):

$$\begin{pmatrix} a \\ c \\ k \\ K \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ k \end{pmatrix}.$$

Thus, any icosahedral quasicrystal may be regarded as a packing of unit cells. Three types of quasicrystals (P, I, F) correspond to three types of tilings, each with its own basis set of unit cells. All three tilings are consistent with the higher-dimensional approach, and the procedure of projecting from six-dimensional space is unambiguous.

All nodes of the P-type quasilattice are a subset of nodes of the I-type quasilattice, which, in turn, are a subset of nodes of the F-type quasilattice. A complete agreement with the theoretically derived values of the inflation factor is achieved: this factor is τ^3 for type P and τ for types I and F [24].

Three versions of packing with global icosahedral symmetry, which are locally isomorphic to each other and are generated according to uniform rules depending on the choice of the initial configuration, exist for each of the three types of quasicrystals. Let us clarify this using type I as an example. If one takes tetrahedron k, multiplies it by the I_h icosahedron group, and groups the resulting 120 copies around vertex A, the first initial configuration is obtained. Two more configurations are obtained in a similar manner (by grouping 120 copies of tetrahedron c around vertex B or 120 copies of tetrahedron K around vertex C). The initial configurations for types P and F are chosen in an equivalent way from similar polyhedra. Therefore, there are always exactly three types of nodes with local icosahedral symmetry (A, B, C) and, as a consequence, three types of characteristic icosahedral clusters both in the zonohedral tiling with inflation factor τ^3 and in two Danzer tilings into different sets of tetrahedra with inflation factor τ.

If all 120 copies of each of the basis tetrahedra (the complete orbit of the cell in group I_h) are filled with atoms in the same way, the resulting structure is centrosymmetric and corresponds to the I_h symmetry group. If, however, at least one of the basis tetrahedra and its mirror copy are considered different, the structure lacks an inversion center and corresponds to the I symmetry group. This type of cell decoration naturally induces the emergence of right and left enantiomorphic forms.

Thus, the theory based on the use of three types of tilings with their unit cells decorated with specific atoms in accordance with the local matching rules is efficient in solving almost all problems of structural design of icosahedral quasicrystals. The concept of unit cells allows one to characterize the structures of icosahedral quasicrystals of all three types (P, I, F) within both symmetry groups (I_h, I); notably, the phenomenon of enantiomorphism may be taken into account in the case of non-centrosymmetric structures. The tiling into zonohedra and two tilings into tetrahedra are fully consistent with each other and with the higher-dimensional approach and, consequently, may be used to refine the structures of quasicrystalline alloys.

Funding

This study was supported by grant No. 23-23-00392 from the Russian Science Foundation (https://rscf.ru/project/23-23-00392/).

Conflict of interest

The author declares that he has no conflict of interest.

References

[1] *Optics of aperiodic structures. Fundamentals and device applications*, ed by L. Dal Negro (Pan Stanford Publ., Singapore, 2014). DOI: 10.1201/b15653

[2] Y. Nagaoka, J. Schneider, H. Zhu, O. Chen, Matter, **6**, 30 (2023). DOI: 10.1016/j.matt.2022.09.027

[3] A. Poddubny, E. Ivchenko, Physica E, **42**, 1871 (2010). DOI: 10.1016/j.physe.2010.02.020

[4] W. Man, M. Megens, P. Steinhardt, P.M. Chaikin, Nature, **436**, 993 (2005). DOI: 10.1038/nature03977

[5] S.Y. Jeon, H. Kwon, K. Hur, Nat. Phys., **13**, 363 (2017). DOI: 10.1038/nphys4002

[6] S. Boriskina, Nat. Photon., **9**, 422 (2015). DOI: 10.1038/nphoton.2015.107

[7] E.G. Noya, C.K. Wong, P. Llombart, J.P.K. Doye, Nature, **596**, 367 (2021). DOI: 10.1038/s41586-021-03700-2

[8] W. Steurer, T. Haibach, in *International tables for crystallography*, ed. by U. Shmueli (Springer, Dordrecht, 2006), vol. B, ch. 4.6, p. 486–532. DOI: 10.1107/97809553602060000568

[9] W. Steurer, S. Deloudi, *Crystallography of quasicrystals. Concepts, methods and structures* (Springer, Berlin—Heidelberg, 2009). DOI: 10.1007/978-3-642-01899-2

[10] M. Baake, U. Grimm, Acta Cryst. A, **76**, 559 (2020). DOI: 10.1107/S2053273320007421

[11] M. Widom, M. Mihalkovi., Isr. J. Chem., **64**, e202300122 (2024). DOI: 10.1002/ijch.202300122

[12] C.L. Henley, Phys. Rev. B, **43**, 993 (1991). DOI: 10.1103/PhysRevB.43.993

[13] A.E. Madison, RSC Adv., **5**, 5745 (2015). DOI: 10.1039/C4RA09524C

[14] A.E. Madison, RSC Adv., **5**, 79279 (2015). DOI: 10.1039/C5RA13874D

[15] A.E. Madison, P.A. Madison, Proc. Roy. Soc. A, **475**, 20180667 (2019). DOI: 10.1098/rspa.2018.0667

[16] A.E. Madison, P.A. Madison, Struct. Chem., **31**, 485 (2020). DOI: 10.1007/s11224-019-01430-w

[17] A.E. Madison, P.A. Madison, V.A. Moshnikov, Tech. Phys., **69**, 528 (2024).

[18] J.E.S. Socolar, P.J. Steinhardt, Phys. Rev. B, **34**, 617 (1986). DOI: 10.1103/PhysRevB.34.617

[19] L. Danzer, Discrete Math., **76**, 1 (1989). DOI: 10.1016/0012-365X(89)90282-3

[20] L. Danzer, Z. Papadopolos, A. Talis, Int. J. Mod. Phys. B, **7**, 1379 (1993). DOI: 10.1142/S0217979293002389

[21] M. Senechal, *Quasicrystals and geometry* (Cambridge University Press, Cambridge, 1995).

[22] L.S. Levitov, J. Rhyner, JETP Lett., **47**, 760 (1988). http://jetpletters.ru/ps/1099/article_16620.pdf.

[23] P. Kramer, Z. Papadopolos, M. Schlottmann, D. Zeidler, J. Phys. A, **27**, 4505 (1994). DOI: 10.1088/0305-4470/27/13/024

[24] P. Kramer, Z. Papadopolos, D. Zeidler, in *Symmetries in science V*, ed. by B. Gruber, L.C. Biedenharn, H.D. Doebner (Springer, Boston, 1991), p. 395–427. DOI: 10.1007/978-1-4615-3696-3_19

Translated by D.Safin