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Archetypes and Other Embeddings of Periodic Nets Generated by Orthogonal Projection

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Archetypes are defined as embeddings of minimal nets with maximal symmetry. A simple geometrical construction is proposed to construct the archetype associated with two-line-connected graphs with more than one cycle and without loops and a criterion is derived to check the embedding. The periodicity of the archetype is equal to the cyclomatic number of the quotient graph of the net, and the factor group of its space group with respect to the normal subgroup of all translations is isomorphic to the automorphism group of the quotient graph. Orthogonal projections are considered to ensure the generation of periodic structures with three-dimensional coordination polyhedra. © 1999 Academic Press

INTRODUCTION

It was shown previously (1) that the framework of various three-periodic structures mapped on isomorphic quotient graphs could be obtained by orthogonal projection of the embedding of a unique (up to isomorphism) n-periodic net mapped on the same quotient graph. This embedding, which was called the archetype, bore the property that the factor group of its space group with respect to the normal subgroup of all translations was isomorphic to the automorphism group of the quotient graph and its periodicity was equal to the cyclomatic number of this graph. Extensive use of group theory, by way of the generators of the automorphism group of the quotient graph, was then made to derive the general form of the archetype. The method involves fastidious calculations and moreover poses the question of the generality of the existence of the archetype since nontrivial symmetry is a fortuitous phenomenon. In this paper, we rely exclusively on graph theory (2) to propose a general algorithm leading to the archetype. A simple criterion is derived which allows checking the embedding. The paper is closed with examples illustrating the necessity of further projection to satisfy three-dimensional coordination around the points of the embedding, thereby providing a physical interpretation for some of the projections involved in obtaining the real structure from the archetype.

INTEGRAL EMBEDDING AND ARCHETYPES

In this section, we introduce *integral embedding* and *archetypes* in the case of the graphite net. The next section generalizes the results by applying graph-theoretical tools. Consider the graph $K_2^{(3)}$ represented in Fig. 1a. Any embedding of a periodic net admitting this graph, as a quotient graph, should display two-point lattices A and B of valence 3 and three line lattices mapped on the three edges AB. We obtain a particularly simple embedding of such a net by setting the line lattices equal to the three vectors $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ of an orthonormal basis of the three-dimensional Euclidian space E^3. This is indicated in Fig. 1a by orienting and labeling the edges of the graph. Note that this is not a labeled quotient graph as this was defined by Chung *et al.* (4). The framework shown in Fig. 1b was generated accordingly, by first placing a point of type A at the origin of E^3 and then drawing from each point of type A or B subsequently obtained three lines AB or BA, parallel or opposite, respectively, to the basis vectors. The procedure must clearly recur indefinitely until an infinite framework is formed. It is apparent that the net associated with this framework is the two-periodic minimal net (3) associated with the graph $K_2^{(3)}$. By construction of the embedding, both kinds of points have integer coordinates; so we call it the integral embedding of the minimal net.

We can choose the vectors $\mathbf{a}$ and $\mathbf{b}$ of E^3 given below, as basis vectors for the two-periodic lattice:

$$\mathbf{a} = \mathbf{e}_1 - \mathbf{e}_2,$$
$$\mathbf{b} = \mathbf{e}_2 - \mathbf{e}_3.$$

It is clear from Fig. 1b that the position vectors $\mathbf{r}(h, k)$ of points of type A or B are given as written below, for any pair (h, k) of integers:

$$\mathbf{r}_A(h, k) = h\mathbf{a} + k\mathbf{b} = h\mathbf{e}_1 + (k - h)\mathbf{e}_2 - k\mathbf{e}_3,$$
$$\mathbf{r}_B(h, k) = \mathbf{e}_1 + h\mathbf{a} + k\mathbf{b} = (h + 1)\mathbf{e}_1 + (k - h)\mathbf{e}_2 - k\mathbf{e}_3.$$

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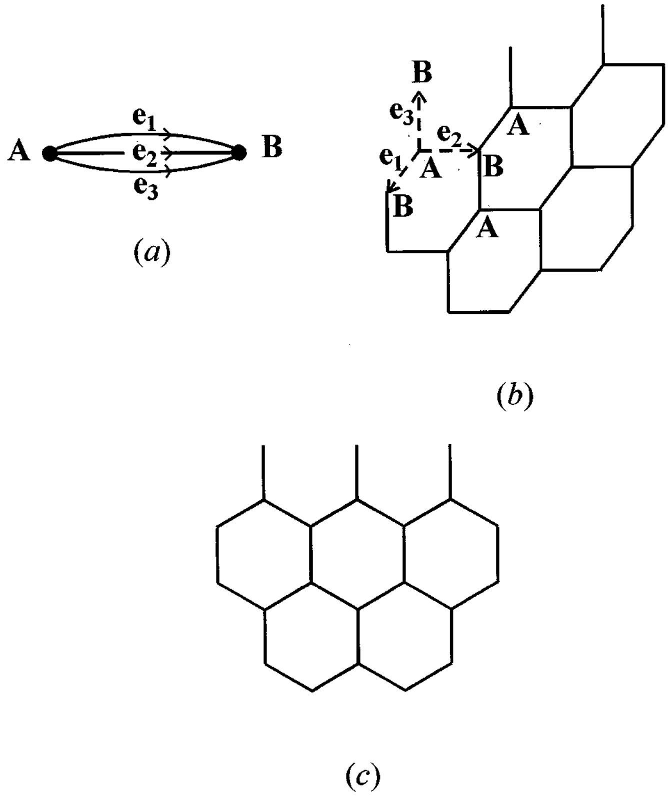

FIG. 1. (a) Graph $K_2^{(3)}$ with (b) the associated integral embedding, and (c) the planar framework 6^3 obtained after projection along the direction [111].

Points of type A and points of type B belong to two parallel planes. Indeed, where the summation is over the index i ($i = 1, 2, 3$) and x_i represent the coordinates of a point in E^3, with $n = 0$ for points of type A and $n = 1$ for points of type B, both satisfy the equation

$$\sum x_i = n. \qquad [1]$$

Conversely, it is easily verified that any point with integer coordinates in these two planes belongs to the corresponding point lattice.

Now, we wish to generate a two-dimensional, two-periodic embedding for the same net; this can be realized by projecting the integral embedding into the plane of any of the point lattices, giving the planar framework 6^3 of the graphite structure represented in Fig. 1c. The embedding is the archetype associated with the graph $K_2^{(3)}$.

GRAPH-THEORETICAL ANALYSIS

Basic concepts of graph theory can be found in Harary (2). Of special importance to this work, however, are the concepts of *cycle space* and *cocycle space*, which have been extended to the field of real numbers, so that we briefly recall their origin hereafter. Definitions of net, embedding, and quotient graph of a net are given in Beukemann and Klee (3) and Chung *et al.* (4).

Let G be a connected graph with possibly loops and multiple edges for which an orientation has been chosen. A 0-*chain* and a *l-chain* of G are formal linear combinations of vertices and edges, respectively, with real coefficients. The *boundary* and *coboundary operators* ∂ and δ are linear operators defined between these two spaces by the following rules:

$\partial e = v - u$, if $e = uv$ is edge oriented from vertex u to vertex v.

$\delta u = \sum \varepsilon_i e_i$, where the sum is over the edges e_i incident with vertex u and $\varepsilon_i = 1$ if e_i is oriented outward from u and $\varepsilon_i = -1$ otherwise.

The *cycle space D* is the kernel of the boundary operator whereas the *cocycle space* Δ is the image space of the coboundary operator.

$x \in D \Leftrightarrow \partial x = 0$.

$y \in \Delta \Leftrightarrow \exists w$: $y = \delta w$, where x and y are 1-chains and w is a 0-chain.

It can be proven that the two spaces D and Δ are completementary in the 1-chain space. The *cyclomatic number* m(G), also called cycle rank (2), is the dimension of the cycle space, i.e., the maximum number of independent cycles of G. If G has p vertices and q edges, then $m(G) = q - p + 1$. The dimension of the cocycle space is thus equal to $p - 1$, and the coboundaries of all but one vertex can be used as a basis of the cocycle space.

The 1-chain space can be given the structure of a Euclidian space if we formally consider the set of edges $\{e_i, i = 1, \ldots, q\}$ as 1-chains forming an orthonormal basis. This basis is called hereafter the natural basis of the graph. It can then be verified that the cycle and cocycle spaces are orthogonal.

Let us have another look at the graph $K_2^{(3)}$ in Fig. 1a. With two vertices and three edges, the cycle space is two-dimensional and the cocycle space is one-dimensional. The 1-chains $e_1 - e_2$ and $e_2 - e_3$ are obviously independent cycles and can be used as a basis for the cycle space. The coboundary $\delta A = e_1 + e_2 + e_3$ is a basis vector of the cocycle space. Let us now identify the 1-chain space of this graph and Euclidian space E^3 that was used to draw the integral embedding, by using the natural mapping:

$$e_i \to \mathbf{e}_i, \quad i = 1, 2, 3.$$

Equation [1] then represents the equation of planes parallel to the cycle space, or orthogonal to the cocycle space. These results are now generalized.

Although no restriction should forbid the presence of vertices of degree 2 in the graph, these can always be eliminated by contraction: we thus consider that G has minimal vertex degree 3. It is known therefore that, up to isomorphism, there is a unique minimal net of periodicity m(G) admiting G as its quotient graph (3). The integral embedding of this net is constructed in E^q, the 1-chain Euclidian space of G, by setting each line lattice equal to the basis vector associated with the respective edge of G. We can choose the origin of E^q at an arbitrary point of some point lattice O. If c_i ($i = 1, \ldots, m$(G)) are independent cycles forming a basis of the cycle space of G, then any linear combination $C = \sum n_i c_i$ with integer coefficients n_i gives the position of a point of point lattice O. These combinations correspond naturally to closed walks in G. Conversely, any 1-chain of G with integer coefficients, which is mapped to zero by the boundary operator ∂, is clearly a closed walk in G, i.e., a linear combination of the basis cycles c_i. Thus, point lattice O can be identified to the set of points of the cycle space that have integer coordinates. The position vectors of the points of any point lattice M are given by $g_M + C$, where g_M is a geodesic linking the vertices O and M in the quotient graph. This reveals that the integral embedding is limited to p m(G)-dimensional affine subspaces parallel to the cycle space, thus being of infinite extension along the cycle space but of finite extension in orthogonal directions, along the cocycle space. The archetype is obtained by projecting the integral embedding along the cocycle space of graph G into its cycle space.

Using the orthogonal projection to generate the archetype ensures obtaining the highest possible symmetry (the aristotype). Indeed, a geometrical interpretation of the projection that maps to the vector null the coboundary δP, that is, that maps to zero the outward sum of the edges adjacent to point lattice P, is that is puts the points of P at the center of their coordination sphere. However, if desired, it is always possible to add some distortion to the embedding by projecting some vectors of the cocycle basis in definite directions of the cycle space. We consider below the example of the perovskite structure.

Figure 2 shows the labeled graph $K_{1,3}^{(2)}$ corresponding to the octahedral skeleton of the perovskite $CaTiO_3$. We first define matrix K whose columns give the coordinates of the basis vectors of the cycle (c_i, $i = 1, 2, 3$) and cocycle (d_i, $i = 1, 2, 3$) spaces in the natural basis:

$$(c_1, \ldots, d_3) = (e_1, \ldots, e_6) \cdot K.$$

$$K = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & 0 & -1 \end{bmatrix}.$$

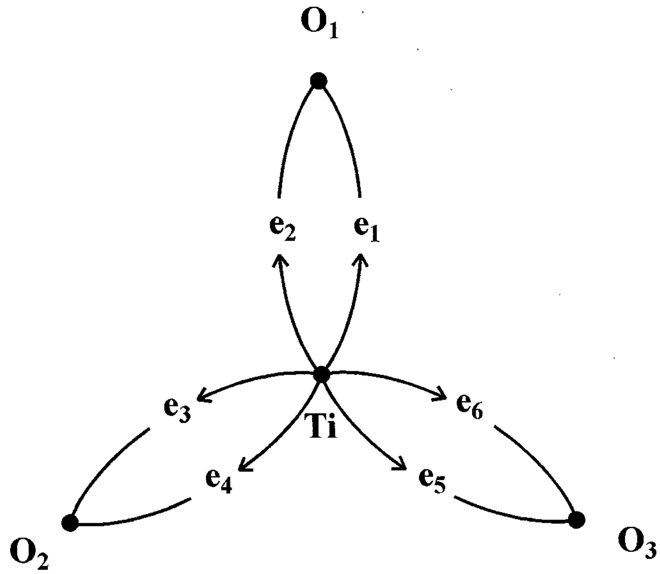

FIG. 2. Graph $K_{1,3}^{(2)}$ for generation of the perovskite structure.

The product of K and its transpose gives the metric tensor Z of the integral embedding:

$$Z = K^t \cdot K = 2 \cdot I_6, \text{ where } I_q \text{ is the unit matrix of } E^q.$$

It follows that the lattice of the integral embedding, and consequently its projection in the cycle space along the cocycle space, are cubic. We define matrix T, describing the projection in the cycle–cocycle basis

$$T = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

The columns of matrix L defined below give the coordinates of the line lattices in the cubic cycle basis:

$$L = T \cdot K^{-1},$$

$$L = \begin{pmatrix} 0.5 & -0.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & -0.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.5 & -0.5 \end{pmatrix}.$$

To introduce a tetragonal distortion in the perovskite framework, we can project the three vectors of the cocycle basis on the first basis vector of the cycle space, for example,

$$T = \begin{pmatrix} 1 & 0 & 0 & 0.04 & 0.02 & 0.02 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix},$$

$$L = \begin{pmatrix} 0.48 & -0.52 & -0.01 & -0.01 & -0.01 & -0.01 \\ 0 & 0 & 0.5 & -0.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.5 & -0.5 \end{pmatrix}.$$

The relative coordinates of the four atoms, calculated from matrix L, are given below; they indicate a shift of the central atom Ti and its two ligands O_1 along the first axis:

$$O_1: 0.49 \quad 0 \quad 0,$$

$$O_2: 0 \quad 0.50 \quad 0,$$

$$O_3: 0 \quad 0 \quad 0.50,$$

$$\text{Ti}: 0.01 \quad 0 \quad 0.$$

In some cases, only partial projection from the cocycle space is required. For example, the graph $P_2^{(2)}$ represented in Fig. 3 corresponds to the quotient graph of the layers in the structure of red mercuric iodide. All that is needed here is to project the two-periodic, four-dimensional integral embedding along one direction to generate a two-periodic, three-dimensional structure. This can be done by projecting along the coboundary vector $\delta\text{Hg} = e_1 + e_2 + e_3 + e_4$ to create tetrahedral coordination around the central atom.

LOOPS AND BRIDGES

The two critical graphs displayed in Figs. 4a and 4b are representative of the embedding inconsistencies that arise from the presence of loops and bridges in the quotient graph. On one hand, we require, as a first criterion for a good embedding, that the distance between any pair of nonbonded points be strictly larger than the length of a line (5). On the other hand, the different bonds (lines) are required to have comparable lengths, which is meant, for the time being, as a fuzzy criterion. In the case of the first graph, Fig. 4a, the integral embedding does not meet the requirements because points A, which are not linked together, are brought to a bonding length in the direction defined by the loop. In the case of the second graph, Fig. 4b, the bridge is orthogonal to both cycles of the graph, i.e., is orthogonal to the cycle space and is therefore null in projection. Two different vertices are consequently superposed in projection, which is not acceptable. We thus restrict the study of quotient graphs to graphs without loops and bridges, i.e., to two-line-connected graphs without loops (2). Note that the special graph with one vertex and an arbitrary number of loops, although trivial, leads to acceptable solutions.

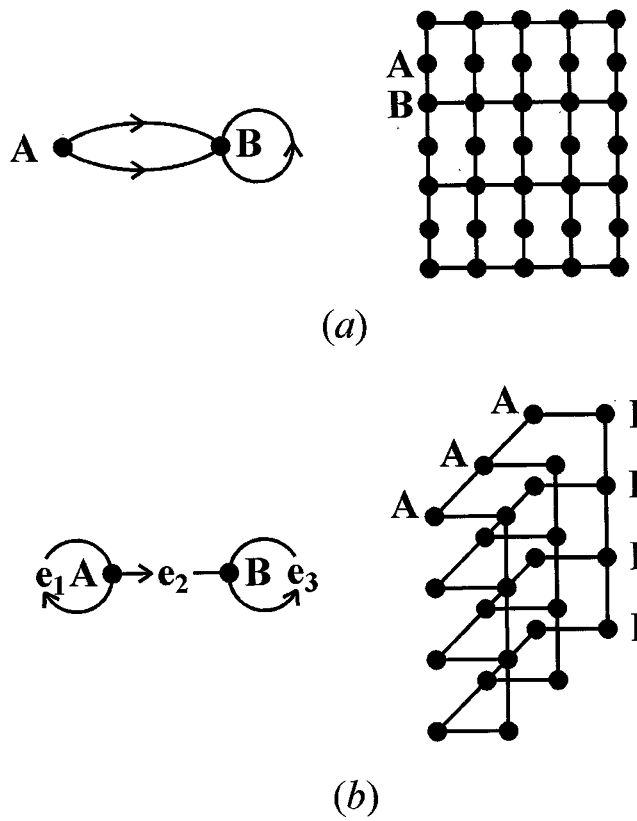

FIG. 4. Typical cases of bad embedding: (a) projection on the cycle space of the integral embedding for a graph with a loop and (b) integral embedding for a graph with a bridge.

By construction, the bonds in the integral embedding have unit length. Now, in a graph without loops, any cycle combines at least two edges, that is, two vectors of the natural basis of the graph. Thus, the norm of any vector of the lattice in E^q is the square root of an integer, at least equal to 2, which means that the requirements for embedding the integral embedding are fulfilled by the points of the same point lattice.

Moreover, it is easily verified that a geodesic between two different vertices A and B of the quotient graph G defines the shortest distance between points of these two-point lattices of the integral embedding. If the geodesic has length n in G, the distance between the extremities of the corresponding path in the integral embedding is the square root of n, which is at least 2, when the point lattices are not linked. We conclude that the integral embedding meets all requirements for embedding whenever the quotient graph does not have loops.

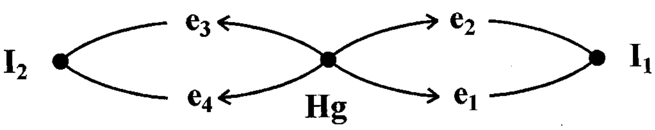

FIG. 3. Graph $P_2^{(2)}$ for generation of the red HgI_2 structure.

A CRITERION FOR THE EMBEDDING OF THE ARCHETYPE

We proceed to examine the properties of the projection of the integral embedding on the cycle space $E^{m(G)}$ when the quotient graph is two-line-connected without loops. Let us first recall that the Voronoi cell $V(x)$ of a lattice Λ at a vertex x is the set of points of $E^{m(G)}$ that lie at least as close to x as to any other point of Λ (6). The facet vectors f form the set F of vectors joining x to another vertex of Λ whose Voronoi cell shares a facet (an n-dimensional face) with $V(x)$. If α is the vector joining x to a point y of $E^{m(G)}$, the following test determines whether y belongs to $V(x)$ (6):

$$\forall f \in \mathrm{F}, \quad 2\alpha \cdot f \leq |f|^2 \qquad [2]$$

In this relation, $\alpha \cdot f$ is the scalar product of the two vectors and $|f|$ is the norm of f.

We now show that any geodesic g of the quotient graph satisfies relation [2] for any cycle f of G. Indeed, we can write in the natural basis, with the summation running over all edges of G:

$$g = \sum g_i e_i \qquad \text{with } g_i \in \{-1, 0, 1\},$$

$$f = \sum n_i e_i \qquad \text{where } n_i \text{ are integers},$$

$$2g \cdot f = 2\sum g_i \cdot n_i \leq 2\sum |g_i \cdot n_i| \leq \sum n_i^2 = |f|.$$

The equality only occurs when the cycle f is the reunion of g and another edge-disjoint geodesic. We observe also that the scalar product of f with the projection $T(g)$ of g on the cycle space $E^{m(G)}$ is equal to the scalar product of f and g, since f is a vector of the cycle space. We thus obtain the result that two points of the projection separated by a path that is mapped to a geodesic in the quotient graph belong to the Voronoi cell associated with any of them.

Let then X and Y be two point lattices of the framework obtained by the projection of the integral embedding on the cycle space, and choose one point x of X. By definition of $V(x)$, the points y of Y which are inside or on a facet of the Voronoi cell $V(x)$ are at least as close to x as to any other point of X. Thus, to see whether the projection meets the first requirement for an acceptable embedding, we only need to compare the distance between x and y, that is, the projection of a geodesic of G from X to Y, with the lengths of the bonds from x and y. It is clear that the points of a same point lattice satisfy this requirement since the respective distances have not changed after projection of the integral embedding on the cycle space.

Let B be the matrix of the projection in the cycle–cocycle basis. It is a diagonal matrix with "1" in the first $m(G)$ entries of the diagonal and "0" in the next $(q - m(G))$ entries. The matrix of the projection in the natural basis is then

$$E = K \cdot B \cdot K^{-1}$$

The squares of the lengths of the lines in the projection are given by the diagonal entries of matrix E. The minimum distance separating two points x and y of point lattices X and Y, linked in G by the geodesic g, is then given by $d(g)$,

$$(d(g))^2 = g^t \cdot E \cdot g,$$

where g is the column vector and g^t its transpose row vector giving the coordinates of the geodesic in the natural basis.

A special case is that of quotient graphs which are complete graphs, K_n, or complete graphs with multiple edges, $K_n^{(m)}$. With the exception of K_2, these graphs are two-line-connected without loops and thus have well-defined integral embeddings. Moreover, the geodesics of the quotient graph correspond to its edges. All requirements for embedding the archetype defined by quotient graphs $K_n^{(m)}$ are then satisfied. Since the q edges of G are equivalent, as is the case for any transitive graph, their lengths $d(e)$ in projection are equal and the sum of their square is the trace of matrix E:

$$q \cdot (d(e))^2 = \mathrm{tr}(E) = \mathrm{tr}(B) = m(G).$$

In the general case, we can use the criterion that the distance given by any geodesic $d(g)$ must be greater than the projection of the lines linked to the extremities of the geodesic $d(e)$:

$$d(g) > d(e). \qquad [3]$$

SPACE GROUPS

We now assume that all embedding requirements are satisfied and examine the q-dimensional space group Γ of the integral embedding. From the position vectors of the points of the embedding, $g_M + C$, as given above, it is clear that the subgroup $\Theta(\Gamma)$ of all translations contained in Γ corresponds exactly to the cycle vectors C. By definition, the automorphisms of the graph G correspond to the permutations of the edges that preserve the adjacency relation (4). These permutations map the corresponding permutations of the vectors of the natural basis of G and thus generate an isomorphic group of linear transformations of E^q. We shall use the same notation for the automorphism of G and the geometrical transformation in E^q. As has already been noted for three-dimensional embeddings (1), it follows from the definitions that the factor group $\Gamma/\Theta(\Gamma)$ of the space group of the integral embedding with respect to the normal subgroup of all translations is isomorphic to a subgroup of the automorphism group Aut(G) of its quotient graph.

Consider an automorphism A of Aut(G), which maps the origin O and an arbitrary vertex M of G to vertices O′ and M′, respectively. We write $[A, g_{O'}]$ for the isometry of E^q with linear component A and translation component $g_{O'}$, which corresponds to a geodesic from O to O′ in G. We now show that this isometry maps the points of point lattice M to points of point lattice M′. By definition of the isometry, we have

$$[A, g_{O'}] \cdot g_M = A \cdot g_M + g_{O'},$$

where $A \cdot g_M$ represents the image by the automorphism A of the geodesic g_M in G; since A preserves the adjacency relation, this is a geodesic from O′ to M′. Adding the geodesic $g_{O'}$, which goes from O to O′, we obtain a walk from O to M′, which is equal to the sum of a geodesic $g_{M'}$ from O to M′ and a cycle c of G, possibly null:

$$[A, g_{O'}] \cdot g_M = g_{M'} + c.$$

The definition of the linear operator A ensures the mapping of the lines crossing at any point of M to the lines crossing at the point of M′ to which this was mapped. This shows that the isometry $[A, g_{O'}]$ maps the integral embedding to itself and belongs to space group Γ. The factor group $\Gamma/\Theta(\Gamma)$ and the automorphism group Aut(G) are thus isomorphic and we have $\Gamma = \{[A, g_{O'} + C]\}$, where A is any automorphism of Aut(G) and C is any closed walk of G, as defined above.

Consider now the m(G)-dimensional space group of the archetype whose points are defined by $B \cdot g_M + C$, where B is the matrix of the projection, as above. It is clear that the group of the translations of the archetype contains all the cycle vectors C of the cycle space. Since a translation of the embedding also maps an automorphism of the quotient graph, there will be no other translation if there is no automorphism of G, other than the identity, which leaves all the cycles fixed.

Let A be such an automorphism; it realizes a circular permutation of the vertices and edges along any cycle. We now show that A is necessarily the identity of Aut(G) if the graph G is two-line-connected and contains more than one cycle. It is clear that this is not true for a graph made of only one cycle, as any circular permutation of its edges leaves the cycle globally invariant.

Let us say that two cycles are tangent if they share a single common vertex or a common set of edges forming a path, as represented in Fig. 5. We first observe that the two kinds of tangent cycles have no nontrivial circular permutation of their edges that leaves both cycles fixed. To complete the proof, we show that any vertex a of a two-line-connected graph which contains more than one cycle belongs to a pair of tangent cycles and is thus fixed by the automorphism.

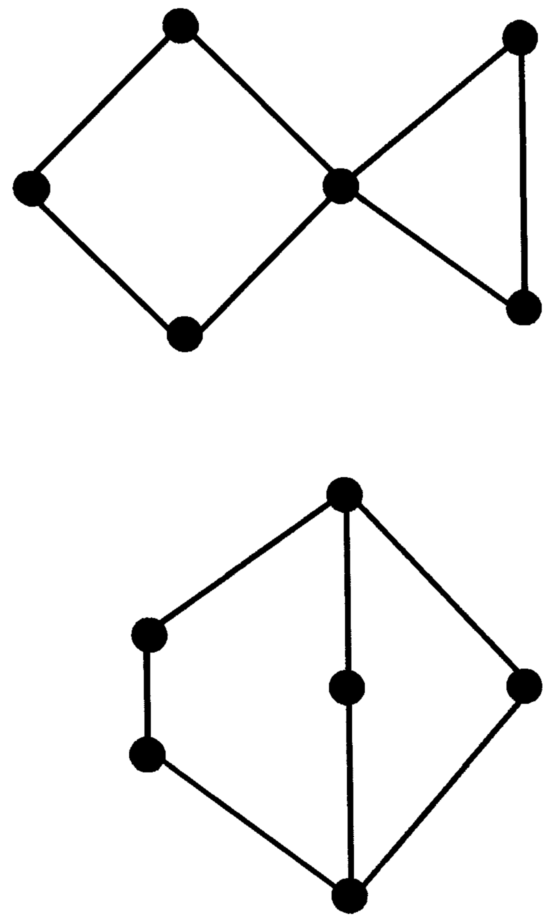

FIG. 5. Tangent cycles.

Let b be any other vertex of G (see Fig. 6). Since G is two-line-connected, there must be at least two line-disjoint paths from a to b (2); let us choose two such paths and form a cycle C_1. As G contains more than one cycle, there is at least another vertex c of G that does not belong to the cycle C_1. Consider now two line-disjoint paths p_1 and p_2 joining

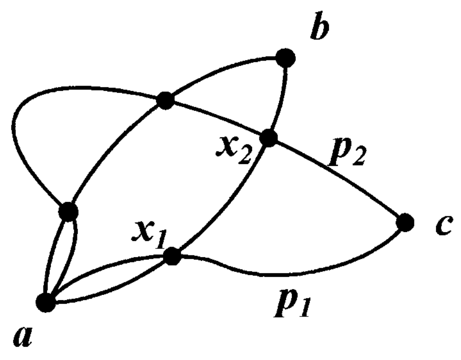

FIG. 6. Construction of a pair of tangent cycles from any vertex a of a two-line-connected graph G with more than one cycle and without loops.

c and a, and the vertices x_1 and x_2 on p_1 and p_2, respectively, which are the first vertices belonging to cycle C_1 encountered when going from c to a. Both x_1 and x_2 may possibly be confounded with a. The two extremities of the paths p_1 and p_2, from x_1 to c and from c to x_2, together with part of the cycle C_1 from x_2 to x_1, form another cycle C_2 which is tangent to C_1. The restriction of the automorphism A to these cycles is therefore the identity of the group $\mathrm{Aut}(C_1 \cup C_2)$, which shows that vertex a is fixed by A.

On one hand, all vertices of G are consequently fixed by A, which implies that the cocycles are fixed. We have already supposed that the cycles are fixed by A; this shows that A is the identify of Aut(G).

On the other hand, since any automorphism of G preserves the adjacency relation, both the cycle and cocycle spaces are stable subspaces in E^q. This means that the linear operator associated in E^q with the automorphism A of Aut(G) and the projection operator B commute. It follows that, for any automorphism A, the restriction of the isometry $[A, B \cdot g_{O'}]$ to the cycle space E^q maps the point lattice $B \cdot g_M + C$ of the archetype to the point lattice $B \cdot g_{M'} + C$,

$$\begin{aligned}[A, B \cdot g_{O'}] \cdot (B \cdot g_M + C) &= A \cdot (B \cdot g_M + C) + B \cdot g_{O'} \\ &= B \cdot (A \cdot g_M + g_{O'}) + A \cdot C \\ &= B \cdot (g_{M'} + c) + A \cdot C \\ &= B \cdot g_{M'} + C',\end{aligned}$$

where $C' = c + A \cdot C$ is a cycle vector of E^q and $g_{M'}$ is the geodesic of G to which the geodesic g_M is mapped by A, as above. By definition of the automorphism, it is clear that line lattices $B \cdot e_i$ too are mapped to line lattices of the archetype, and thus that the restriction to the cycle space of the isometry $[A, B \cdot g_{O'}]$ belongs to the space group of the archetype. Now, we have seen that, for a graph with more than one cycle, there is no automorphism of G, other than the identity, which leaves all the cycles fixed. Thus, the restrictions of the operators A to the cycle space form a group which is isomorphic to the automorphism group Aut(G). In that case, the space group of the projection along the cocycle space and that of the integral embedding are isomorphic.

We conclude that whenever the projection along the cocycle space of the integral embedding of the minimal net associated with a two-line-connected graph G with more than one cycle and without loops satisfies the embedding requirements, the factor group $\Gamma/\Theta(\Gamma)$ of the space group of the projection with respect to the normal subgroup of all translations is isomorphic to the automorphism group Aut(G) of the quotient graph G of the net: this justifies the identification of this projection to the archetype N[G].

COORDINATION CONSTRAINTS

The graph $K_2^{(6)}$ represented in Fig. 7 corresponds to the quotient graph of the NaCl structure. The vector labels obtained by the program TOPOLAN (7) have been introduced in the graph conjointly with the formal labeling of the edges in E^6. In accordance with the previous arguments, the archetype $N[K_2^{(6)}]$ is a well-defined five-dimensional embedding. The coordination polyhedron around both kinds of points of this framework is the regular hexatope (8), i.e., the regular polytope with six vertices of E^5. Octahedral coordination can be generated through projection of the hexatope in three-dimensional space. Using the labeling indicated in Fig. 7, we may informally require pairing of opposite edges to define the octahedral coordination:

$$a + b = c + d = e + f (= 0).$$

These equations turn out to involve the three-dimensional lines obtained after projection of the hexatope. So they are not to be applied in this form to the respective vector labels from TOPOLAN since their terms are not cycles of the quotient graph. However, we observe that two independent cycles, C_1 and C_2, can be generated from the formal combination, as 1-chains, of the corresponding edges of the quotient graph:

$$C_1 = a - c + b - d,$$

$$C_2 = a - e + b - f.$$

The sum of the vector labels from TOPOLAN of the quotient graph of the NaCl structure along these cycles is clearly null. It is thus possible to project the archetype along the plane spanned by these two cycle vectors to derive the NaCl structure.

The fluorite structure, the labeled quotient graph $P_2^{(4)}$ of which is shown in Fig. 8, provides another simple example. The application of relation [3] to the only nontrivial geodesic $g = e - a$ shows that the archetype $N[P_2^{(4)}]$ is a well-defined six-dimensional embedding. The edges must,

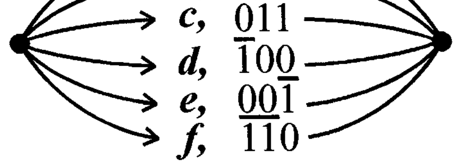

FIG. 7. Labeled quotient graph $K_2^{(6)}$ of the NaCl structure.

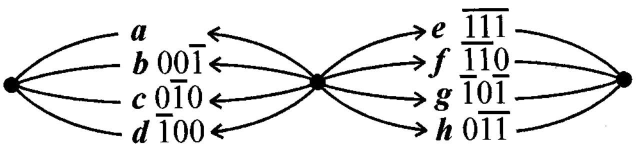

FIG. 8. Labeled quotient graph $P_2^{(4)}$ of the fluorite structure.

however, verify the following relations to satisfy cubic coordination:

$$a + e = b + f = c + g = d + h (= 0).$$

The fluorite net is accordingly obtained through projection of the archetype $N[P_2^{(4)}]$ along the three-dimensional subspace spanned by the cycle vectors C_1, C_2, and C_3:

$$C_1 = a - b + e - f,$$

$$C_2 = b - c + f - g,$$

$$C_3 = c - d + h - g.$$

The rutile net with the labeled quotient graph shown in Fig. 9 is more representative of the general phenomenon. After the criterion for embedding based on relation [3] is applied to the three nontrivial (and not symmetry-equivalent) geodesics g_1, g_2, and g_3, we can check that the archetype is a well-defined seven-dimensional embedding:

$$g_1 = a_1 - b_1,$$

$$g_2 = a_1 - a_3,$$

$$g_3 = a_1 - a_5.$$

The coordination polyhedron around both Ti points in E^7 is a distorted hexatope. Octahedral coordination can be obtained through projection of the archetype by pairing the edges informally as follows:

$$a_1 + a_4 = a_2 + a_3 = a_5 + a_6,$$

$$b_3 + b_5 = b_4 + b_6 = b_1 + b_2.$$

Therefore, we introduce four 1-chains of the quotient graph:

$$\sigma_1 = a_1 + a_4 - a_2 - a_3,$$

$$\sigma_2 = a_1 + a_4 - a_5 - a_6,$$

$$\sigma_3 = b_3 + b_5 - b_4 - b_6,$$

$$\sigma_4 = b_3 + b_5 - b_1 - b_2.$$

It turns out that σ_1 and σ_3 are cycles of the graph but not the other two. However, by applying the boundary operator ∂ to σ_2 and σ_4, we find

$$\partial\sigma_2 = -\partial\sigma_4 = O_1 + O_2 - O_3 - O_4$$

which shows that the 1-chain $\sigma_2 + \sigma_4$ belongs to the cycle space of the quotient graph. Moreover, it can be checked that the 1-chain $\sigma_2 - \sigma_4$ belongs to the cocycle space of the graph and was already projected onto the vector null in deriving the archetype. Accordingly, the projection of the archetype along the three-dimensional subspace spanned by the three cycle vectors σ_1, σ_3, and $\sigma_2 + \sigma_4$ produces a four-dimensional embedding with octahedral (three-dimensional) coordination around the Ti points. It can be seen in Fig. 9 that the results are in agreement with the vector labeling of the rutile quotient graph as it is obtained from TOPOLAN: the sum of the vector labels along σ_1, σ_3, and $\sigma_2 + \sigma_4$ is null.

The method can now be generalized. To define the projecting subspace of the cycle space leading to three-dimensional coordination polyhedra, one writes the 1-chains obtained from expressing the relations between the lines crossing at each point in the three-dimensional space. The

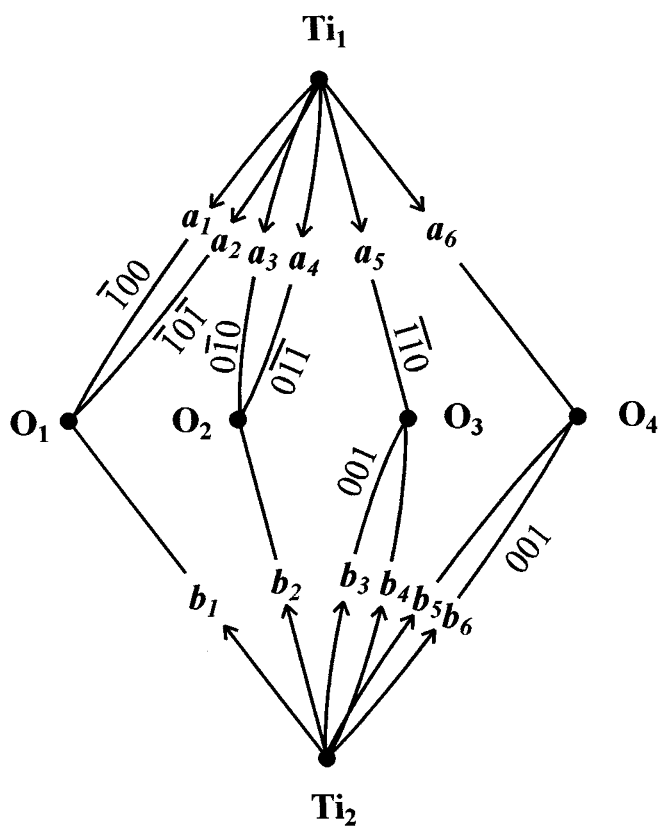

FIG. 9. Labeled quotient graph of the rutile structure.

cycle vectors spanning the projection subspace can be obtained by looking for integer combinations of these 1-chains that belong to the kernel of the boundary operator.

CONCLUSION

Archetypes are defined as $m(\mathrm{G})$-periodic embeddings of minimal nets with maximal symmetry. Their periodicity is equal to the cyclomatic number $m(\mathrm{G})$ of their quotient graph G and their point group; that is, the factor group of their space group with respect to the normal subgroup of all translations is isomorphic to the automorphism group of this graph. The paper describes a geometrical construction showing the existence of the archetype associated with two-line-connected graphs with more than one cycle and without loops. For a graph with p vertices and q edges, the cycle and cocycle spaces are defined as complementary subspaces in the Euclidian space E^q. An embedding of the minimal net is constructed that is periodic along the cycle space but has finite extension along the cocycle space and then projected on the cycle space. A simple criterion allows for checking the embedding of the archetype. In general, it is necessary to define further projections along some subspace of the cycle space to obtain a three-dimensional coordination polyhedron around each point of the framework. Whether other projections that are needed to draw real three-dimensional structures from the archetype could eventually be given some physical interpretation is an open question.

Finally, we observe that the symmetry point group of the framework projected from the archetype should be isomorphic to the subgroup of the automorphism group of the quotient graph that leaves the subspace defining the projection invariant.

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