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Tilings by hexagonal prisms and embeddings into primitive cubic networks

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All possible combinatorial embeddings into primitive cubic networks of arbitrary tilings of 3D space by pairwise congruent and parallel regular hexagonal prisms are discussed and classified.

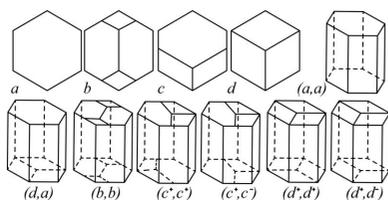
1. Introduction

We discuss all (not necessarily face-to-face) tilings of the 3D Euclidean space by mutually congruent and parallel regular hexagonal prisms. The main result is as follows: if the graph of such a tiling contains cycles of only even length, then it can be embedded combinatorially into a primitive cubic network (**pcu** net) of dimension 3 or 4. Embeddings of three indecomposable parallelohedra (rhombic and elongated dodecahedra and the truncated octahedron) are represented as embeddings of appropriate tilings by prisms. A criterion for right prism tiling of the 3D space is presented by Schulte & Ivić Weiss (1997).

This study contributes to the research on modelling crystal growth and crystal complexity using finite automata (Mackay, 1976; Krivovichev, 2014). Development of automata that model crystal growth can be achieved through embedding the periodic graph of the crystal into a **pcu** net. Embeddings of face-to-face tilings by parallelohedra and applications for building structural automata that model the growth of periodic structures were studied by Bouniaev & Krivovichev (2020).

In this study, we address the challenge of the 3D **pcu** net being too 'tight' for some tilings. For example, although the graph of the rhombic dodecahedron cannot be embedded into the 3D **pcu** net, it is embeddable into the 4D **pcu** net. Mapping 2D or 3D combinatorial structures into high-dimensional **pcu** nets was proposed by S. Novikov in the 1980s, and developed by N. Dolbilin, M. Shtan'ko and M. Shtogrin in a series of studies, including the report by Dolbilin *et al.* (1995).

We define the graph of an arbitrary tiling T of 3D space by convex polyhedral cells. Let x be a point of the space, and denote by $i(x)$ the number of all cells of T that contain x and by $F(x)$ the intersection of those (closed) cells. If $i(x) = 1$, then $F(x)$ is a cell of T that contains x . If $i(x) = 2$, then $F(x)$ is a convex polygon called a *face* of the tiling T . Furthermore, if $n(x) \geq 3$, then $F(x)$ is either a single point called a *vertex* of T , or a segment called an *edge* of the tiling. This set of vertices and edges of a tiling T is called a *graph* G of T . For face-to-face tiling T , our definition of a graph G of T coincides with the standard definition of the edge graph of a tiling T . We say that graph G is *embeddable* into a **pcu** net if there is a subgraph in



the graph of the **pcu** net that is combinatorially isomorphic to G .

Let us describe all tilings by mutually congruent and parallel regular hexagonal prisms. We assume that the hexagonal bases of the prisms are positioned in horizontal planes.

In addition to the face-to-face tiling, there are two disjoint classes of such tilings. In a tiling, if there is a prism whose lateral face is shared by more than one adjacent prism, then a hexagonal base of any prism is shared by only two prisms in the tiling. This tiling is called a *tiling with vertical shift* and denoted by T_v . In contrast, if there is a prism whose horizontal base is shared by more than one adjacent prism, then any lateral face is shared by exactly two prisms of the tiling. Such a tiling is called *tiling with horizontal shift* and denoted by T_h .

The necessary condition for embedding a graph into a **pcu** net is that the graph must contain cycles of even length only. Note that the graph of the face-to-face tiling by hexagonal prisms is uniquely embeddable into the 3D **pcu** net.

2. Tilings with vertical shift

In a T_v , all prisms are grouped in vertical columns. The lateral edge of a prism can be subdivided by at most 2 vertices of T_v located in the interior of the edge. The lateral edge of a prism is of type k , $k = 0, 1, 2$, if there are k vertices of the tiling in its interior.

Theorem 2.1. If T_v has even cycles only, then the lateral edges of all prisms are of the same type k , and $k \neq 0$. For $k = 2$, the graph of T_v is combinatorially unique. For $k = 1$, there are infinitely many combinatorial types of graphs of T_v .

Case $k = 0$ corresponds to the face-to-face tiling.

If $k = 2$, each prism can be surrounded by adjacent prisms in combinatorially unique way.

If $k = 1$, there are five and only five combinatorial types of surrounding P by adjacent prisms. The resulting structures are represented by the Schlegel diagrams in Fig. 1. The lateral face of the prism shared by two adjacent prisms is partitioned in Fig. 1 into two cells by a dotted line. The prism can be decorated by dotted lines in five approaches, numbered 1a–1e.

It can be easily verified that the respective graphs in Figs. 1 and 2 are isomorphic as stated in Theorem 2.2.

Theorem 2.2. The graph of a T_v is embeddable into the 3D **pcu** net. As shown in Fig. 2, the graphs of types 1a and 1b can be uniquely embedded. The graphs of types 1c, 1d, 1e and 2 can be embedded in two ways. The graphs of types 1c and 2 are isomorphic to the graphs of the elongated dodecahedron and truncated octahedron, respectively.

3. Tilings with horizontal shift

In a T_h , all hexagonal prisms are grouped in the bi-infinite sequence of layers $\dots L_{-1}, L_0, L_1, \dots$ separated by planes $\Pi_i = L_{i-1} \cap L_i$. All lateral edges of each prism in T_h remain as edges of a graph G of T_h .

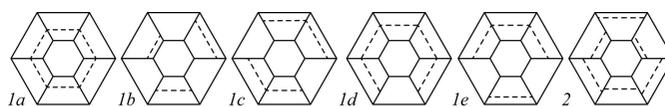


Figure 1 Schlegel diagrams for type 1a–1e and type 2 prisms.

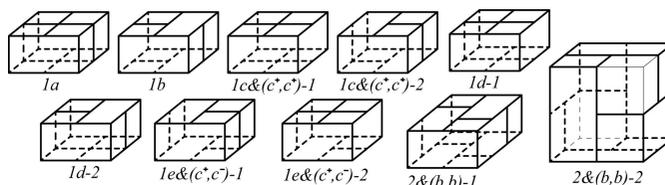


Figure 2 Embeddings of prisms from T_v and T_h .

The edges and vertices of G that lie in a plane Π_i form a subgraph $G_i = G \cap \Pi_i$. The structure of G_i is determined by the relative shift between the two adjacent layers L_{i-1} and L_i . For a prism $P \subset L_i$, there are prints of graphs G_{i+1} and G_i on its hexagonal bases. Owing to the evenness condition, only the following combinatorial types of hexagons with prints are possible: a, b, c, d (Fig. 3). We say that P is a *decorated prism* of type (p, q) if p is the type of subgraph G_i in plane Π_i and q is the type of G_{i+1} in plane Π_{i+1} . It is obvious that all prisms in each layer L_i are of the same type (p, q) . Types c and d can occur in two approaches denoted by c^+ and c^- , and d^+ and d^- , respectively, (Fig. 3).

It can be easily shown that, owing to the evenness of the cycles, the types of decorated prism are as follows (see Fig. 3):

$$(a, a), (a, d^\pm) [\text{or } (d^\pm, a)], (b, b), (c^\pm, c^\pm), (d^\pm, d^\pm). \quad (1)$$

The following combinatorial types of decorated prisms are equivalent: (p, q) and (q, p) , if (p, q) is in list (1), (c^+, c^+) and (c^-, c^-) , (d^+, d^+) and (d^-, d^-) , (d^+, a) and (d^-, a) .

Tiling T_h , whose graph contains only even cycles, corresponds to some bi-infinite sequence $C(T_h)$ consisting of shift types a, b, c^\pm, d^\pm , where any pair (p, q) of consequent types is in list (1). We call the sequence $C(T_h)$ a *code* of T_h .

All possible bi-infinite sequences with all consequent pairs from list (1) can be classified into the following families:

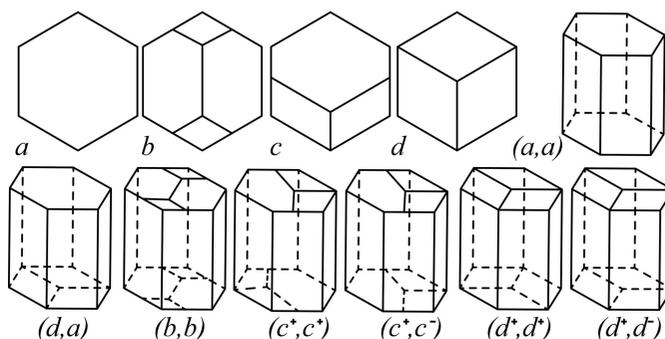


Figure 3 Decorated hexagonal faces and prisms.

(i) \mathcal{C}_b consists of sequences with at least one element b . Because in list (1) b is paired only with itself, this family consists of the sequence $\dots b, b, b, \dots$.

(ii) \mathcal{C}_c consists of sequences where one of the terms is either c^+ or c^- . Because in list (1) symbols c^\pm are paired with themselves only, the family \mathcal{C}_c consists of uncountably many sequences of the form $\dots c^+, c^+, c^-, c^+, c^- \dots$.

(iii) \mathcal{C}_d consists of sequences where one of the terms is either d^+ or d^- . In list (1), d^\pm are paired with either d^\pm or a . Therefore, \mathcal{C}_d consists of uncountably many sequences of the form $\dots d^-, a, d^-, d^+, a, d^-, a \dots$. Note that in a subgraph G_i of type d^\pm , there are vertices incident to eight edges of graph G . Therefore, a graph of T_v with the code from \mathcal{C}_d cannot be embedded into the 3D **pcu** net. However, it is embeddable into the 4D **pcu** net.

Theorem 3.1. (i) The graph of a tiling T_h is embeddable into a **pcu** net of dimension 3 or 4, if and only if its code $C(T_h)$ belongs to one of the three families $\mathcal{C}_b, \mathcal{C}_c, \mathcal{C}_d$. (ii) Let $C(T_h) \in \mathcal{C}_b$, the graph of the (b, b) prism is isomorphic to the graph of the truncated octahedron. The sequence from \mathcal{C}_b encodes the graph of the tiling by the truncated octahedron. The graphs of the (b, b) prism and of the corresponding tiling are embedded into the 3D **pcu** net in two ways [Fig. 2, 2&(b, b)-1&2]. (iii) Let $C(T_h) \in \mathcal{C}_c$, the graph of the (c^+, c^+) prism is isomorphic to the graph of the elongated dodecahedron. The codes $\dots c^+, c^+, c^+ \dots$ and $\dots c^-, c^-, c^- \dots$ determine the graph of the tiling by the elongated dodeca-

hedron that is embedded into the 3D **pcu** net in two ways [Fig. 2, 1c&(c⁺, c⁺)-1&2]. The code $\dots c^-, c^+, c^-, c^+ \dots$ determines the graph of the tiling by some dodecahedron that is a cell of the isohedral tiling. The graph can be embedded into the 3D **pcu** net in two ways [Fig. 2, 1e&(c⁺, c⁻)-1&2]. The remaining codes from \mathcal{C}_c determine the graphs of tilings that are uniquely embeddable into the 3D **pcu** net. (iv) Let $C(T_h) \in \mathcal{C}_d$, the graph of the (d^+, d^+) or (d^-, d^-) prism is isomorphic to the graph of the rhombic dodecahedron. The codes $\dots d^+, d^+, d^+ \dots$ and $\dots d^-, d^-, d^- \dots$ determine the graph of the tiling by the rhombic dodecahedron. The graph of the (d^+, d^-) prism is isomorphic to the graph of some dodecahedron that is a cell of the isohedral tiling. The graphs of these dodecahedra and the tiling with any code \mathcal{C}_d cannot be embedded into the 3D **pcu** net; however, they all are uniquely embeddable into the 4D **pcu** net.

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