Nets and Tiling

Michael O'Keeffe

Introduction to tiling theory
and its application to crystal nets

Arizona State University
Start with tiling in two dimensions.

Surface of sphere and plane

Sphere is two-dimensional. We require only two coordinates to specify position on the surface of a sphere:

The coordinates of

Berkeley  37.9 N, 122.3 W

Tempe    33.4 N, 121.9 W
As far as we are concerned

Tilings in two dimensions are edge-to-edge (each edge is common to just two tiles)

In three dimensions face-to-face (each face common to just two tiles)
Three different embeddings of the same abstract tiling

brick wall  
\(c2mm\)

honeycomb  
\(p6mm\)

herringbone  
\(p2gg\)
Again, two embeddings of the same abstract tiling

double brick

Cairo tiling

Both have same symmetry, $p4gm$. The Cairo conformation is the minimum density for equal edges.
Recall Steinitz theorem

Planar 3-connected graph is graph of a convex polyhedron
Tilings of the sphere (polyhedra) - regular polyhedra.
one kind of vertex, one kind of edge, one kind of face

3.4.3.4
3.5.3.5

Quasiregular polyhedra: one kind of vertex, one kind of edge
Tiling of the plane - regular tilings
one kind of vertex, one kind of edge, one kind of face

3\textsuperscript{6} hexagonal lattice
4\textsuperscript{4} square lattice
6\textsuperscript{3} honeycomb net

quasiregular
one kind of vertex, one kind of edge
3.6.3.6 kagome net
honey comb net is not a lattice

A lattice is a set of points related by translations

honeycomb net is actually a *lattice complex*

- a set of symmetry-related points related by translations
cubic Archimedean polyhedra - one kind of vertex

- rhombic-cuboctahedron (rco) $3.4^3 [3^8.4^{18}]$
- snub cube (snc) $3^4.4 [3^32.4^6]$
- truncated tetrahedron (tte) $3.6^2 [6^4.4^4]$
- cuboctahedron (cuo) $3.4\cdot3.4 [3^8.4^6]$
- truncated octahedron (tro) $4.6^2 [4^6.6^8]$
- truncated cube (tcu) $3.8^2 [3^8.8^6]$
- truncated cuboctahedron (tco) $4.6.8 [4^{12}.6^8.8^6]$
icosahedral Archimedean polyhedra - one kind of vertex

- **truncated dodecahedron**
  - tdo $3.10^2 [3^{20}.10^{12}]$

- **truncated icosahedron**
  - tic $5.6^2 [5^{12}.6^{20}]$

- **rhombic-icosidodecahedron**
  - ric $3.4.5.4 [3^{20}.4^{30}.5^{12}]$

- **snub dodecahedron**
  - snd $3^4.5 [3^{80}.5^{12}]$

- **truncated-icosidodecahedron**
  - tid $4.6.10 [4^{30}.6^{20}.10^{12}]$
8 Archimedean tilings

Picture is from O'Keeffe & Hyde Book
Duals of two-dimensional tilings vertices $\leftrightarrow$ faces

dual of octahedron $3^4$
is cube $4^3$
dual of cube $4^3$
is octahedron $3^4$
dual of dual is the original
tetrahedron is self-dual
Duals:
edges <-> faces

The dual of a dual is the original
tetrahedron is self-dual
Duals of 2-D periodic nets

3⁶ ↔ 6³

AlB₂

4⁴ ↔ 4⁴

self-dual
Important terms:

**Polyhedron** convex solid with planar faces has a planar three-connected graph.*

**Simple** polyhedron all vertices trivalent

**Simplicial** polyhedron all faces triangles

Simple and simplicial polyhedra are duals of each other.

*We will call non-convex solids, maybe with divalent vertices, *cages*. 
self-dual nets in crystal structures
see O'Keeffe & Hyde book for many more!

SrMgSi (PbCl$_2$) one of the most-common ternary structure types net and dual (same net displaced) alternate
Euler equation and genus.

For a (convex) polyhedron with

\[ V - E + F = 2 \]
Euler equation and genus.

For a plane tiling with, per repeat unit

$\nu$ vertices
$e$ edges
$f$ faces

$\nu - e + f = 0$
Euler equation and *genus*.

For a tiling on a surface of genus $g$, with, per repeat unit

- $v$ vertices
- $e$ edges
- $f$ faces

$v - e + f = 2 - 2g$

The surface of a body with $g$ holes has genus $g$
genus of a surface

sphere $g = 0$

torus $g = 1$

plane $g = 1$

double torus $g = 2$

note all vertices $4^4$ just like square lattice
knotted torus still has $g = 1$
genus of a net = cyclomatic number of quotient graph

repeat unit of \textbf{pcu}

quotient graph

cyclomatic number = 3

genus of \textbf{pcu} net is 3
Two interpenetrating pcu nets

The $P$ minimal surface separates the two nets. Average curvature zero Gaussian curvature neg.
infinite polyhedra – tilings of periodic surfaces

$4^3.6$ tiling of the $P$ surface ($g = 3$)

4-coordinated net \textbf{rho} (net of framework of zeolite \textbf{RHO})

for the polyhedron $v = 48, e = 96, f = 44, v - e + f = -4 = 2 - 2g$

3-periodic net has vertex symbol $4.4.4.6.8.8$
tilings of $P$ surface ("Schwarzites")
— suggested as possible low energy polymorphs of carbon
Tiling in 3 dimensions

Filling space by generalized polyhedra (cages) in which at least two edges meet at each vertex and two faces meet at each edge. Tilings are “face-to-face”
Tiling that carries the diamond (dia) net
The tile (adamantane unit) is a cage with four 3-coordinated and six 2-coordinated, there are four 6-sided faces i.e. $[6^4]$
Tiles other than the adamantane unit for the diamond net (These are not *proper* – they have lower symmetry)

half adamantane

double adamantane = "congressane"

the arrows point to vertices on a 6-ring that is not a tile face

note 8-ring (not a strong ring)
We have seen that if a net has a tiling at all, it has infinitely many made by joining or dividing tiles. The tiling by the adamantane unit appears to be the “natural” tiling for the diamond net. What is special about it? It fits the following definition:

The **natural tiling** for a net is composed of the smallest tiles such that:

(a) the tiling conserves the maximum symmetry. (**proper**)  
(b) all the faces of the tiles are strong rings.

Notice that not all strong rings are necessarily faces. A net may have more than one tiling that fits these criteria. In that case we reject faces that do not appear in all tilings.

V. A. Blatov, O. Delgado-Friedrichs, M. O’Keeffe, D. M. Proserpio  
natural tiling for body-centered cubic (bcu)

one tile

blue is 4-ring face of tile = essential ring
red is 4-ring (strong) not essential ring
Simple tiling
A simple polyhedron is one in which exactly two faces meet at each edge and three faces meet at each vertex.
A simple tiling is one in which exactly two tiles meet at each face, three tiles meet at each edge and four tiles meet at each vertex (and the tile is a simple polyhedron).
They are important as the structures of foams, zeolites etc. The example here is a tiling by truncated octahedra which carries the sodalite net (sod) (Kelvin structure).
natural tiling of a complex net - that of the zeolite paulingite

PAU
The same tile can produce more than one tiling. Here the congressane (double adamantane) tile is used to form two different tilings that carry the diamond net. (But notice the symmetry of the tilings is lower than that of the net so they are not *proper* tilings).
Flags

regular tilings are flag transitive

2-D flag
vertex-edge-2D tile

3-D flag
vertex-edge-face-3D tile
Regular tilings and Schlafli symbols

(a) in spherical (constant positive curvature) space,
(b) euclidean (zero curvature) space
(c) hyperbolic (constant negative curvature) space

i.e. in $S^d$, $E^d$, and $H^d$ ($d$ is dimensionality)

H. S. M. Coxeter 1907-2003
Regular Polytopes, Dover 1973
The Beauty of Geometry, Dover 1996
Start with one dimension.
Polygons are the regular polytopes in $S^1$
Schläfli symbol is $\{p\}$ for $p$-sided

$\triangle \square \pentagon \hexagon$

$\{\infty\}$ is degenerate case - an infinite linear group of line segments. Lives in $E^1$
Two dimensions. The symbol is \{p,q\} which means that q \{p\} meet at a point three cases:

\[
\text{case (a) } \frac{1}{p} + \frac{1}{q} > \frac{1}{2} \rightarrow \text{tiling of } S^2
\]

\{3,3\} tetrahedron
\{3,4\} octahedron
\{3,5\} icosahedron
\{4,3\} cube
\{5,3\} dodecahedron
Two dimensions. The symbol is \( \{p,q\} \) which means that \( q \{p\} \) meet at a point three cases:

**case (b) \( \frac{1}{p} + \frac{1}{q} = \frac{1}{2} \) → tiling of \( \mathbb{E}^2 \)**

\( \{3,6\} \) hexagonal lattice
\( \{4,4\} \) square lattice
\( \{6,3\} \) honeycomb lattice complex
Two dimensions. The symbol is \( \{p,q\} \) which means that \( q \{p\} \) meet at a point infinite number of cases:

\text{case (c) } 1/p + 1/q < 1/2 \rightarrow \text{tiling of } H^2

any combination of \( p \) and \( q \) (both >2) not already seen

\{7,3\} \quad \{8,3\} \quad \{9,3\}

space condensed to a Poincaré disc
Three dimensions. Schlafli symbol \{p,q,r\} which means \(r \{p,q\}\) meet at an edge.

Again 3 cases

**case (a) Tilings of \(S^3\) (finite 4-D polytopes)**

\{3,3,3\} simplex  
\{4,3,3\} hypercube or tesseract  
\{3,3,4\} cross polytope (dual of above)  
\{3,4,3\} 24-cell  
\{3,3,5\} 600 cell (five regular tetrahedra meet at each edge)  
\{5,3,3\} 120 cell (three regular dodecahedra meet at each edge)
Three dimensions. Schläfli symbol \{p,q,r\} which means \(r \{p,q\}\) meet at an edge.

Again 3 cases

case (b) Tilings of \(E^3\)

\{4,3,4\} space filling by cubes self-dual

Only regular tiling of \(E^3\)
So what do we use for tilings that aren't regular?

Delaney-Dress symbol or D-symbol (extended Schläfli symbol)

Introduced by Andreas Dress (Bielefeld) in combinatorial tiling theory.

Developed by Daniel Huson and Olaf Delgado-Friedrichs.
tile for **pcu**.
one kind of chamber
D-size = 1
D-symbol
<1.1:1 3:1,1,1,1:4,3,4>

tile for **dia**.
two kinds of chamber
D-size = 2
D-symbol
<1.1:2 3:2,1 2,1 2,2:6,2 3,6>
How do you find the natural tiling for a net?

Use TOPOS

How do you draw tilings?

Use 3dt

We ordinary people use face data for tilings
3dt converts them to D symbols.
See next slide:
TILING
NAME "srs"
GROUP I4132
FACES 10
0.12500 0.12500 0.12500
-0.12500 0.37500 0.12500
-0.12500 0.62500 0.37500
-0.37500 0.62500 0.62500
-0.37500 0.37500 0.87500
-0.12500 0.37500 1.12500
0.12500 0.12500 1.12500
0.37500 0.12500 0.87500
0.37500 -0.12500 0.62500
0.12500 -0.12500 0.37500
END

D-symbol

<1.1:10 3:2 4 6 8 10,10
3 5 7 9,6 5 4 10 9,2
10 9 8 7:10,2 2 3,10>

tile for srs net
To calculate D-size

The number of chambers in each tile = $4 \times \frac{\text{number of edges}}{\text{order of point symmetry}}$

Tiling by cubes with 12 edges and symmetry $m-3m$ (order 48)
D-size = $4 \times \frac{12}{48} = 1$

Diamond tile has 12 edges, symmetry $-43m$
D-size = $4 \times \frac{12}{24} = 2$
Transitivity

Let there be $p$ kinds of vertex, $q$ kinds of edge, $r$ kinds of face and $s$ kinds of tile. Then the transitivity is $pqrs$.

Unless specified otherwise, the transitivity refers to the natural tiling.

We shall see that there are five natural tilings with transitivity 1111; these are tilings of the regular nets. (There are at least two not-natural tilings with transitivity 1111 – these have natural tilings with transitivity 1121 and 1112 respectively)
A **dual tiling** tiling is derived from the original by centering the old tiles with new vertices, and connecting the new vertices with new edges that go through each old face. The dual of a dual tiling is the original tiling. If a tiling and its dual are the same it is **self dual**.

The dual of a tiling with transitivity \(pqrs\) is \(srqp\).

The dual of a natural tiling may not be a natural tiling. If the natural tiling of a net is self-dual, the net is **naturally self dual**.

The faces (essential rings) of a natural tiling of a net are **catenated** with those of the dual.
Duals (cont)
The number of faces of a dual tile is the coordination number of the original vertex. The number of vertices of a face of a dual tile is the number of tiles meeting at the corresponding edge of the original tiling. The dual of a simple tiling is thus a tiling by tetrahedra (four 3-sided faces)

Sodalite (sod) tile part of a simple tiling

Dual tiling (blue) is bcu-x 14-coordinated body-centered cubic. A tiling by congruent tetrahedra
Simple tiling again

The dual of a tiling by tetrahedra may not be a simple tiling by simple polyhedra.

Here is an example – the graph of the tile is 2-connected.
(3-coordinated, but not 3-connected!)

net is bcr

This tiles fills space just by translations alone.
Tiling symmetry is R-3.
Some examples of dual structures

simple tiling  tiling by tetrahedra
sodalite (sod) body-centered cubic
type I clathrate (mep) A15 (Cr$_3$Si)
type II clathrate (mtn) MgCu$_2$
Cr$_3$Si (A15)

Type I clathrate melanophlogite (MEP)
Weaire-Phelan foam
examples of duals

diamond (dia) is naturally self dual

the dual of body-centered cubic (bcu) is the 4-coordinated NbO net (nbo)
Tilings by tetrahedra: there are exactly
9 topological types of isohedral (tile transitive) tilings
117 topological types of 2-isohedral (tile 2-transitive)

In all of these there is at least one edge where exactly
3 or 4 tetrahedra meet. Accordingly none of them have
embeddings in which all tetrahedra are acute (dihedral
angles less than $\pi/2$).
What do we know about tilings?

1. Exactly 9 topologically-different ways of tiling space by one kind of tetrahedron

Duals are simple tilings with one kind of vertex. These include the important zeolite framework types SOD, FAU, RHO, LTA, KFI and CHA.

Two of the remaining three (sod-a and hal) have 3-membered rings. The other has many 4-rings.

**wse** not suitable for a silica zeolite
Example of isohedral tiling by tetrahedra (Somerville tetrahedra). Only one that is also vertex transitive. So the dual structure is the only vertex- and tile-transitive simple tiling (transitivity $1121$).

Vertices are body-centered cubic.

Dual structure (sodalite). "Kelvin structure"
Another example: isohedral tiling by half-Somerville tetrahedra

Dual structure - zeolite RHO
The 1-skeleton (net) of RHO is also the 1-skeleton of a $4^3.6$ tiling of a 3-periodic surface.
Yet another isohedral tiling by tetrahedra

12 tetrahedra forming a rhombohedron

Fragment of dual structure
Zeolite structure code **FAU**
(faujasite) - billion dollar material!
Also a $4^3.6$ tiling of a surface
Isohedral simple tilings.

1. Enumerate all simple polyhedra with N faces (plantri - Brendan McKay ANU, Canberra)

2. Determine which of these form isohedral tilings

<table>
<thead>
<tr>
<th>Faces</th>
<th>tilers</th>
<th>tilings</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;14</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>14</td>
<td>10</td>
<td>23</td>
</tr>
<tr>
<td>15</td>
<td>65</td>
<td>136</td>
</tr>
<tr>
<td>16</td>
<td>434</td>
<td>710</td>
</tr>
</tbody>
</table>

The 23 isohedra simple tilings with 14-face tiles
What's this?

A monotypic (but tile 4-transitive) simple tiling by a 14-face polyhedron. Triclinic! P-1 RCSR symbol \textbf{rug}

D symbol for rug

D-size = 576

4.36.4

transitivity

24 48 32 4
How to find edge-transitive nets?

A net with one kind of edge has a tiling that is dual to a tiling with one kind of face.

So let's systematically enumerate all tilings with one kind of face. (faces can be two sided like a coin)

1. list all polyhedra with one kind of face
2. extend the faces with divalent vertices
3. see if the cages form proper tilings

Examples of \([6^4]\) face-transitive tiles
Table 1. Edge-transitive nets retrieved in this study listed by size of the Delaney-Dress symbol (D-symbol) of the proper tiling with smallest size. The 3-letter symbols are the RCSR (http://rcsr.anu.edu.au/) symbols.

<table>
<thead>
<tr>
<th>D-symbol size</th>
<th>uninodal</th>
<th>binodal</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><strong>pcu</strong></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td><strong>bcu, dia, fcu, nbo</strong></td>
<td><strong>flu</strong></td>
</tr>
<tr>
<td>3</td>
<td><strong>reo, sod</strong></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td><strong>crs, hxg</strong></td>
<td><strong>ftw</strong></td>
</tr>
<tr>
<td>6</td>
<td><strong>acs</strong></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td><strong>rhr</strong></td>
<td><strong>bor, mgc, nia, ocu, rht, she, soc, spn, tbo, the, toc, ttt, twf,</strong></td>
</tr>
<tr>
<td>10</td>
<td><strong>lcs, lvt, lcy, srs</strong></td>
<td><strong>ith, scu, shp, stp</strong></td>
</tr>
<tr>
<td>12</td>
<td><strong>lcv</strong></td>
<td><strong>alb, pto</strong></td>
</tr>
<tr>
<td>14</td>
<td><strong>qtz</strong></td>
<td><strong>pts</strong></td>
</tr>
<tr>
<td>16</td>
<td><strong>bcs</strong></td>
<td><strong>sqc</strong></td>
</tr>
<tr>
<td>20</td>
<td><strong>thp</strong></td>
<td><strong>csq, ssa, ssb</strong></td>
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<tr>
<td>24</td>
<td><strong>ana</strong></td>
<td><strong>gar, iac, ibd, pyr, ssc</strong></td>
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<td>28</td>
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<tr>
<td>32</td>
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<td><strong>ctn, pth</strong></td>
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