When is a crystal graph not crystallographic?

Olaf Delgado-Friedrichs

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Answer: when it has “too much symmetry”.

More precisely: when its automorphism group is not a crystallographic space group.

(Crystallographic nets and their quotient graphs, W. E. Klee 2004.)
A crystalline material. What might be its atomic structure?
X-ray crystallography produces something like this.
Adding bonds (or ligands) yields a periodic graph or *net*.
We can discover further structure in this graph . . .
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Crystal nets

Crystallographic groups

Tutte's barycentric embedding

Unstable nets

Automorphisms to isometries

Periodicity fine print

Thanks

... which could lead us into the hyperbolic plane ...
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... or towards a complete partitioning of space.
A *net* is a (3-) connected, locally finite periodic graph.
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A 2-dimensional net, which happens to be planar.
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A 2-dimensional net, which happens to be planar.
A *crystallographic (space) group* is a discrete group of motions in euclidean space with a bounded fundamental domain.

Crystallographic groups are just the ones that generate unbounded, discrete footprint patterns.
Tutte’s idea for drawing graphs “nicely”:

Place a vertex $v$ in the \textit{barycenter} of its neighbors:

$$\sum_{w \in \text{Neighbors}(v)} \text{position}(w) - \text{position}(v) = 0$$
For finite graphs, prescribe a convex outer face.

For polyhedral graphs, this ensures convex drawings. *(How to draw a graph, W. T. Tutte 1963.)*
For periodic graphs, prescribe a vertex lattice.

The solution is then unique, so all periodic barycentric placements are the same up to affine transformations.
An *unstable* net is one with colliding barycentric vertex positions.

Two non-crystallographic and one crystallographic net, all unstable.

But can non-crystallographic nets be stable?
If \( p: G \to \mathbb{R}^n \) is barycentric and \( \varphi: G \to G \) an automorphism, then \( p \circ \varphi \) is also barycentric.

Define affine map \( \alpha_\varphi: \mathbb{R}^n \to \mathbb{R}^n \) with \( \alpha_\varphi(p(v_i)) = p(\varphi(v_i)) \) for just enough vertices \( v_i \in V(G) \) to make it unique.

If \( p \) and \( p \circ \varphi \) are periodic, then \( \alpha_\varphi \circ p = p \circ \varphi \) everywhere.
Because we have finitely many edge lattices, there can up to translations only be finitely many such $\alpha_\varphi$.

By a standard trick (averaging the inner product), we can turn them all into rigid motions, a.k.a. isometries.

Thus $\varphi \mapsto \alpha_\varphi$ defines a group homomorphism that maps $\text{Aut}(G)$ onto a crystallographic group.

If $G$ is stable, the kernel must be trivial.
How could $p$ be periodic, but not $p \circ \varphi$?

For an abstract graph $G$, we must explicitly pick a translation group $T \leq \text{Aut}(G)$.

If $G$ is not crystallographic, $T$ is not unique and we can have $\varphi T \varphi^{-1} \neq T$.

But $p$ was only constructed to be periodic with respect to $T$, not necessarily $\varphi T \varphi^{-1}$. 
Possible ways forward:

– Show uniqueness of barycentric placements under weaker conditions.

– Construct the homomorphism onto a crystallographic group without requiring $\alpha_\varphi$ to be a global match.

– Learn more about the structure of non-crystallographic nets (c.f. work by Eon and Moreira de Oliveira).
That’s all folks!

Further reading:

Slides:
http://gavrog.org/order-order.pdf