What is a Quasicrystal?

Mathematical Foundations of Quasicrystallography

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Introduction

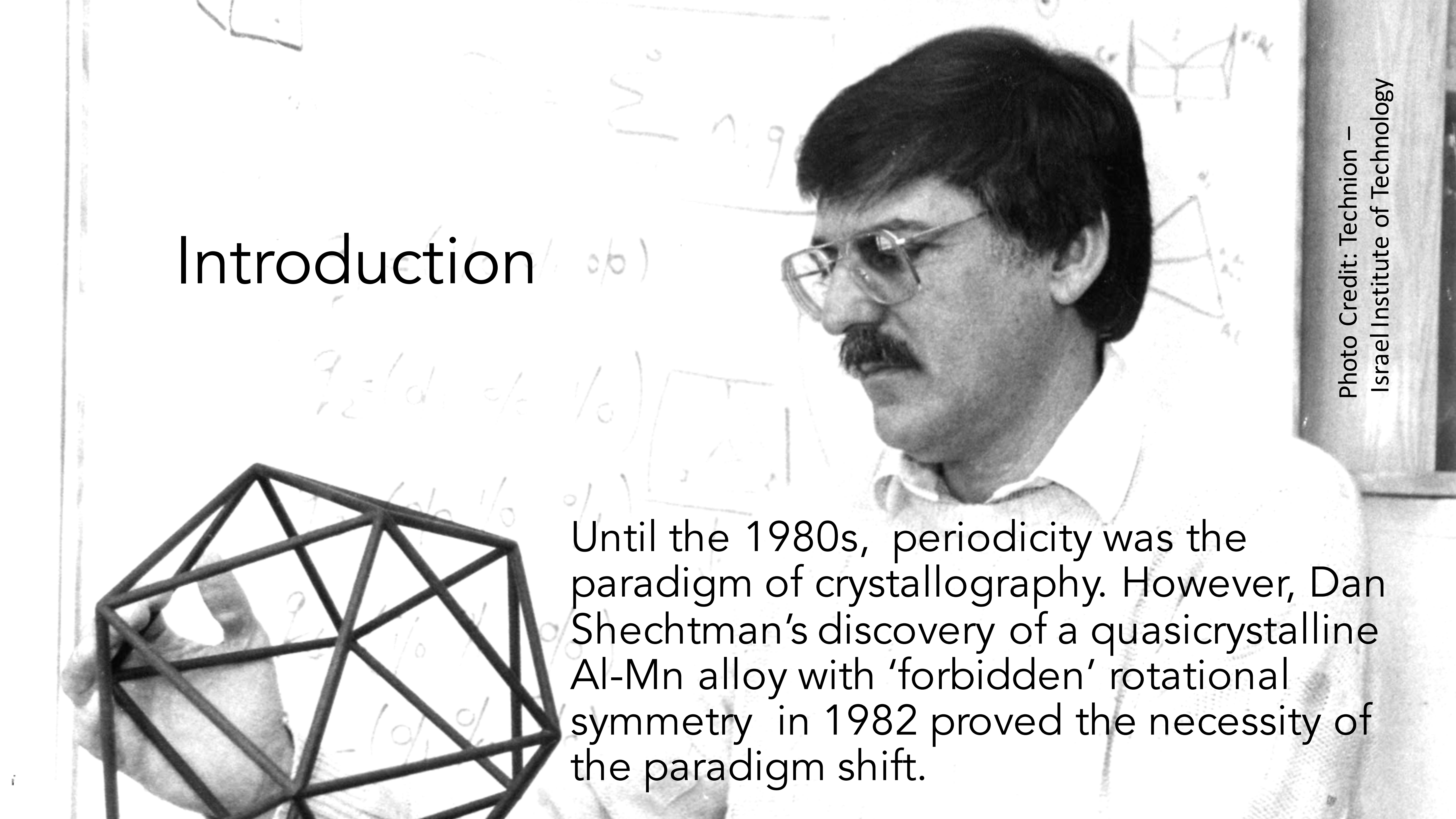


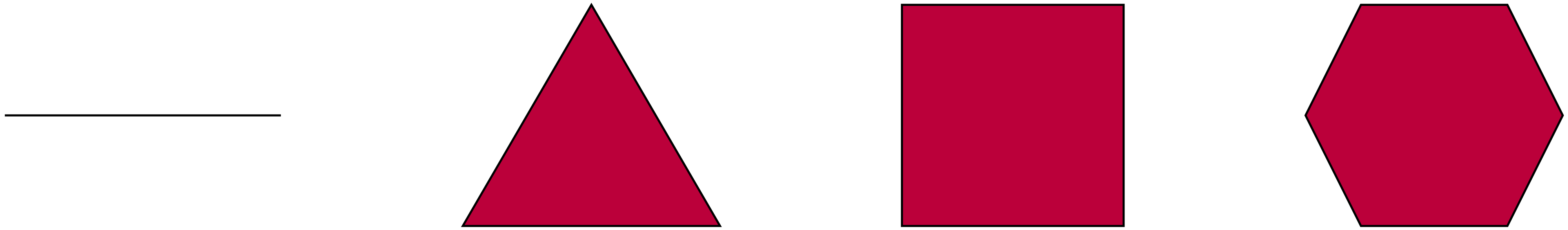
Photo Credit: Technion – Israel Institute of Technology

Until the 1980s, periodicity was the paradigm of crystallography. However, Dan Shechtman’s discovery of a quasicrystalline Al-Mn alloy with ‘forbidden’ rotational symmetry in 1982 proved the necessity of the paradigm shift.

Rotational Symmetry

A point set X is said to possess **rotational symmetry** if X is invariant under the group of rotations.

In two and three dimensions, only 2-fold, 3-fold, 4-fold, and 6-fold rotational symmetries exist. These symmetries are called *crystallographic*.

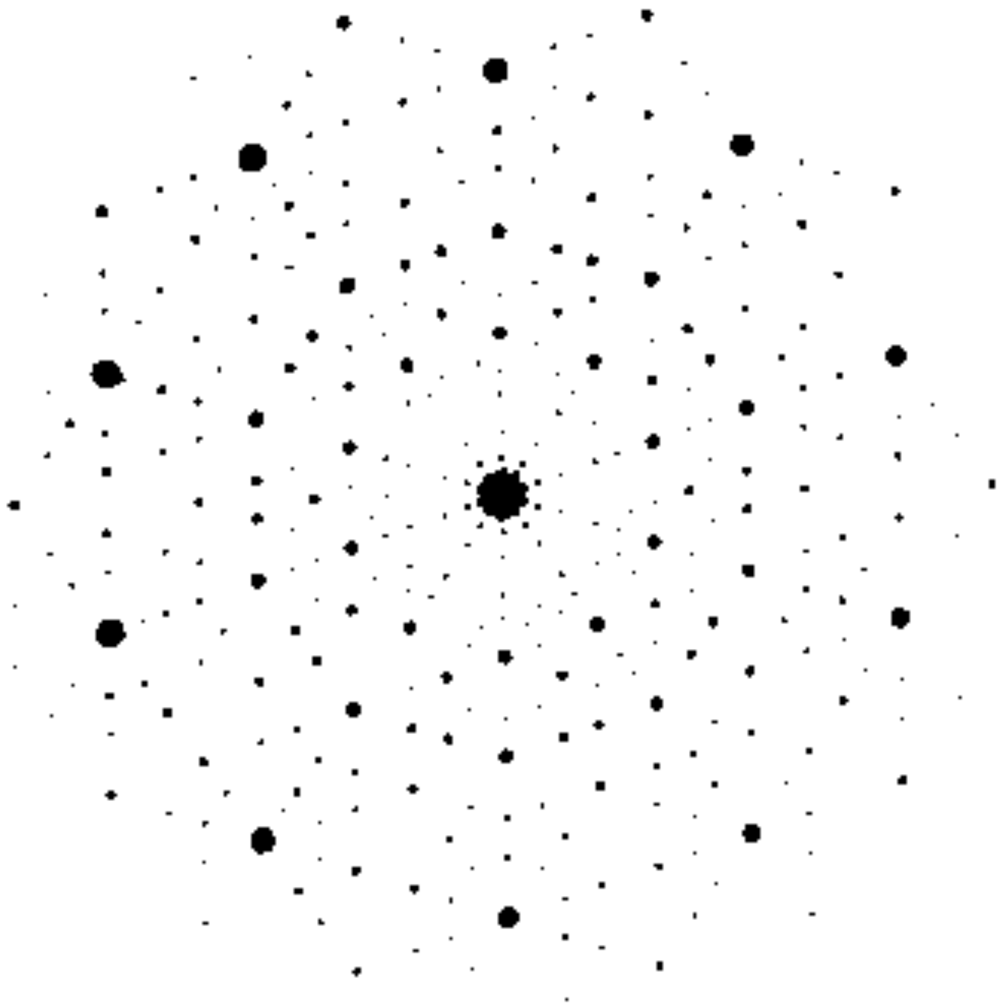


Periodic Structures

Periodic structures in R^n are modelled as lattices spanned by a set of n linearly independent vectors.

The characteristic property of periodic structures is the presence of a **translational symmetry**.

Rotational Symmetry of Periodic Structures



Credit: Shechtman et al, "Metallic phase with long-range orientational order and no translational symmetry"

Periodic structures can only possess crystallographic symmetries.

In 1982 Dan Shechtman discovered an ordered rapidly quenched Al-Mn alloy with the icosahedral point group symmetry. The structure of the alloy was ordered *and* nonperiodic.

Questions

The term *quasicrystal* was coined to describe nonperiodic structures with long-range orientational order but lacking translational symmetry.

However, what *is* a crystal?

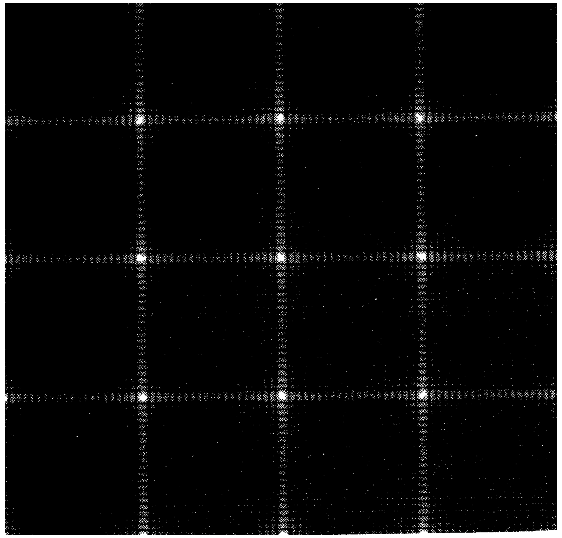
And *what* are quasicrystals and *how* can they be described?

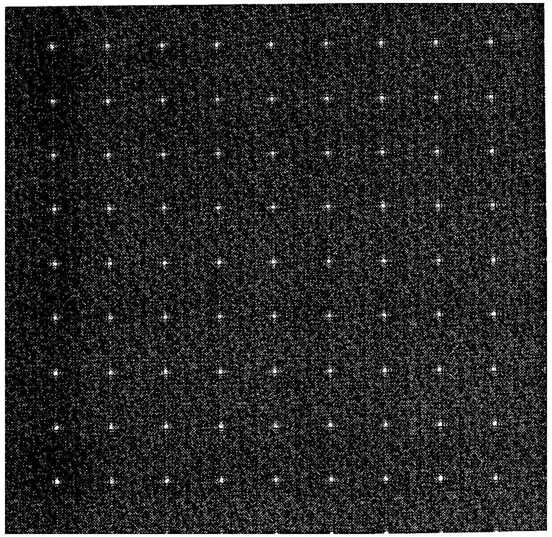
What is the relation between periodicity and aperiodicity?

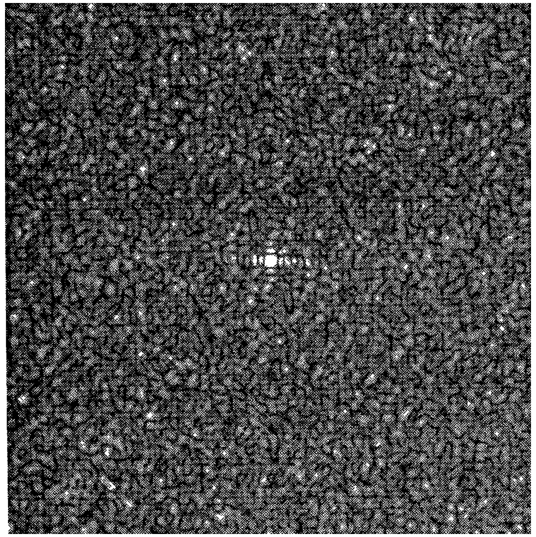
What is the general procedure allowing to construct nonperiodic structures with long-range orientational order?

Paradigm Shift

In 1992 the definition of a crystal was changed by the International Union of Crystallography through the Ad Interim Commission on Aperiodic Crystals. A crystal was defined as *"any solid having essentially discrete diffraction diagram"*.



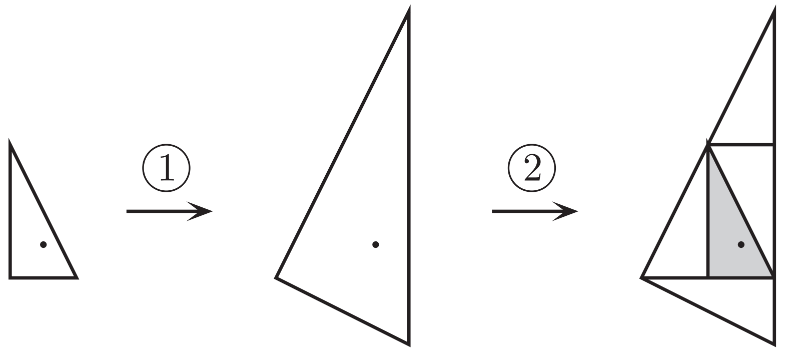


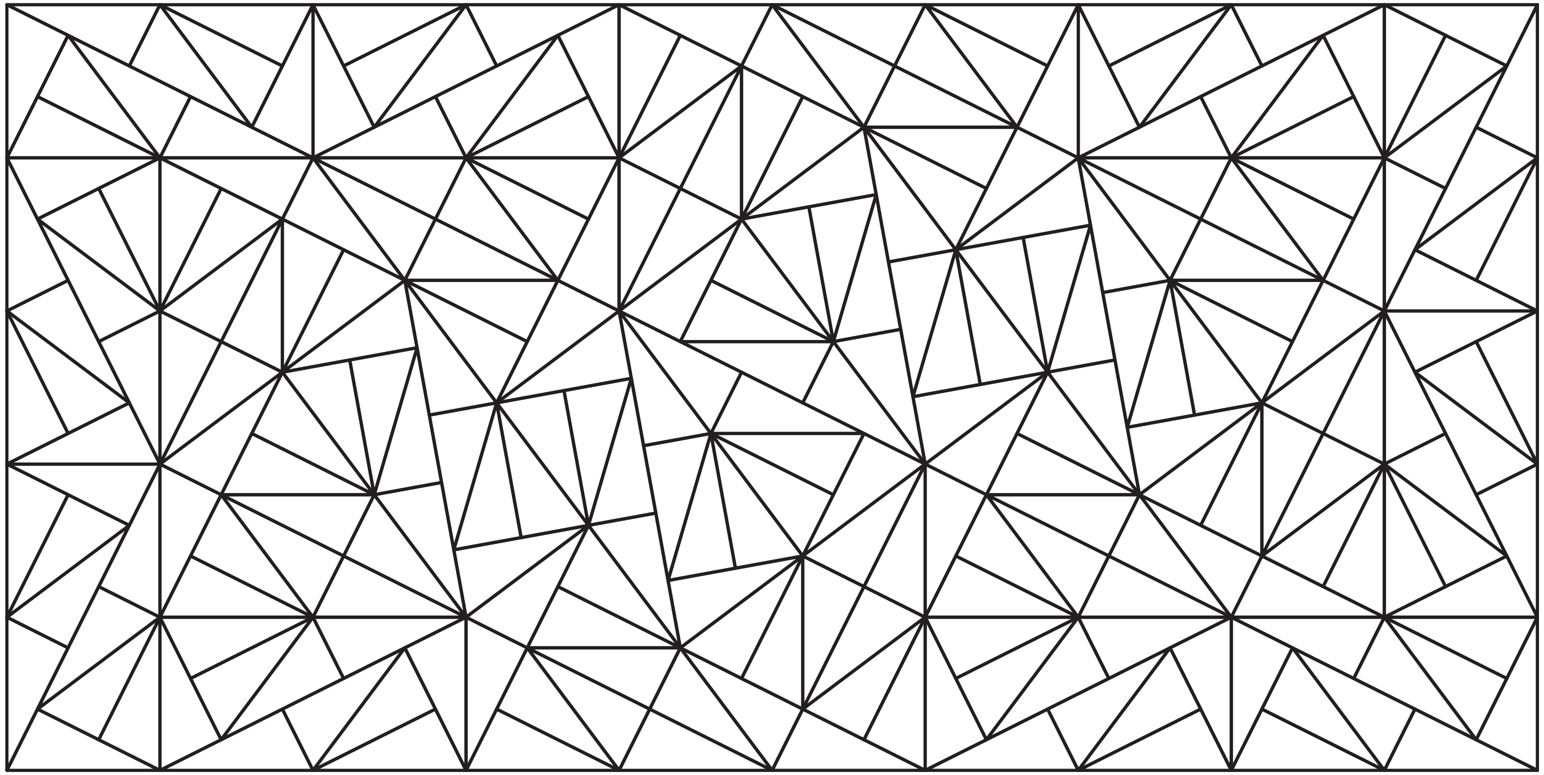


Credit: M.Senechal, "Quasicrystals and Geometry"

Counterexamples

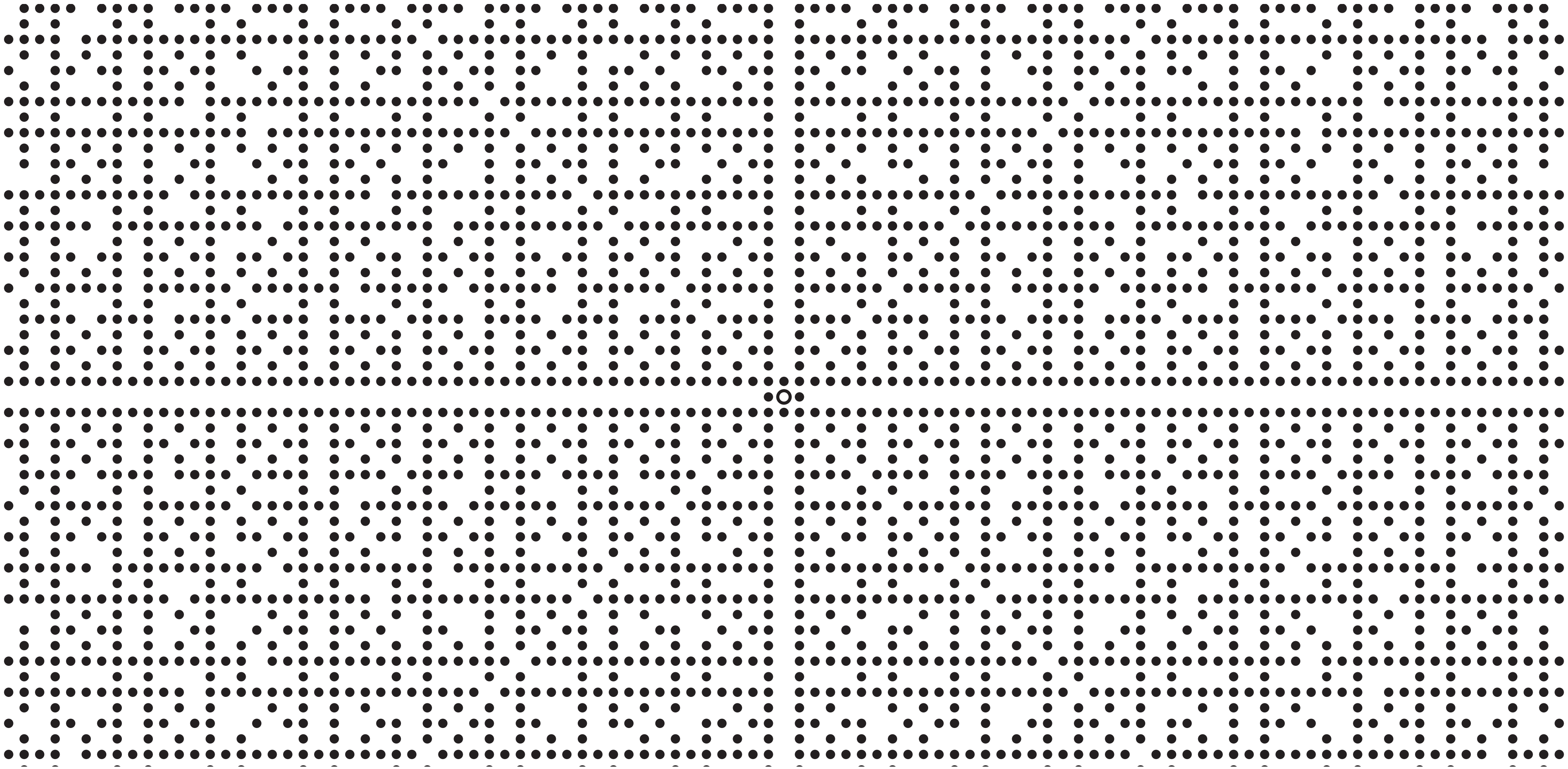
- Pinwheel Tiling





Credit: Baake and Grimm, Aperiodic Order: Volume 1 , A Mathematical Invitation 2013

- Visible Points Lattice



Credit: Baake and Grimm, Aperiodic Order: Volume 1 , A Mathematical Invitation 2013

Modelling Periodic and Nonperiodic Crystals

- Functions

Density functions describe a distribution of points in space and define its diffraction pattern.

- Tilings

A finite set of prototiles corresponds to a finite number of atomic or molecular configurations of a physical crystal.

Modelling Periodic and Nonperiodic Crystals: Measures

- The general framework of measures includes functions and tilings as special cases.
- Almost periodic measures describe both periodic and nonperiodic distributions.
- Diffraction pattern is completely determined by a well-defined measure.

What is a Crystal?

- The definition of a crystal depends on the tools describing its structure.

- In terms of measures, a mathematical crystal can be defined as a distribution of points with a unique autocorrelation measure containing a discrete component.

What is a Quasicrystal?

- A quasicrystal is an abbreviation for a *quasiperiodic crystal.*
- Quasiperiodicity and periodicity are special cases of almost periodicity.
- An almost periodic point set is defined as a point set which distribution can be expanded as a superposition of a countable number of plane waves.
- A point set is called quasiperiodic if there is a finite number of plane waves which define its distribution. Hence, all periodic point sets are quasiperiodic.
- A crystal is called quasiperiodic if and only if its distribution is quasiperiodic.

Construction of Nonperiodic Crystals

- No general procedure encompassing all distinct cases has been developed.

- Known methods include the following:

1. Cut-and-project
2. Multigrid
3. Substitution
4. Matching rules

Further Research

- Rigorous general systematic approach to the study of periodic and aperiodic structures is required.
- The theory of matching rules should be rigorously developed, and the cut-and-project method should be generalised and formalised.
- The inverse problem of homometry is important for the classification of nonperiodic structures.

Evaluation

- Lack of mathematical maturity has delimited the use of available resources.
- Research is largely based on reviews and discussions rather than proofs and arguments.
- No exhaustive and rigorous treatment of the modelling techniques is given.