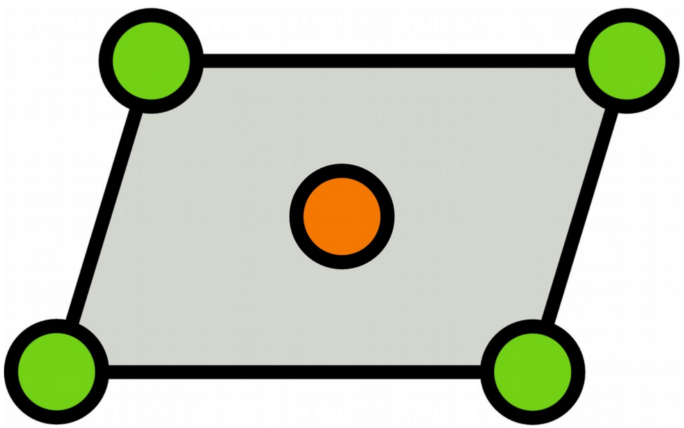
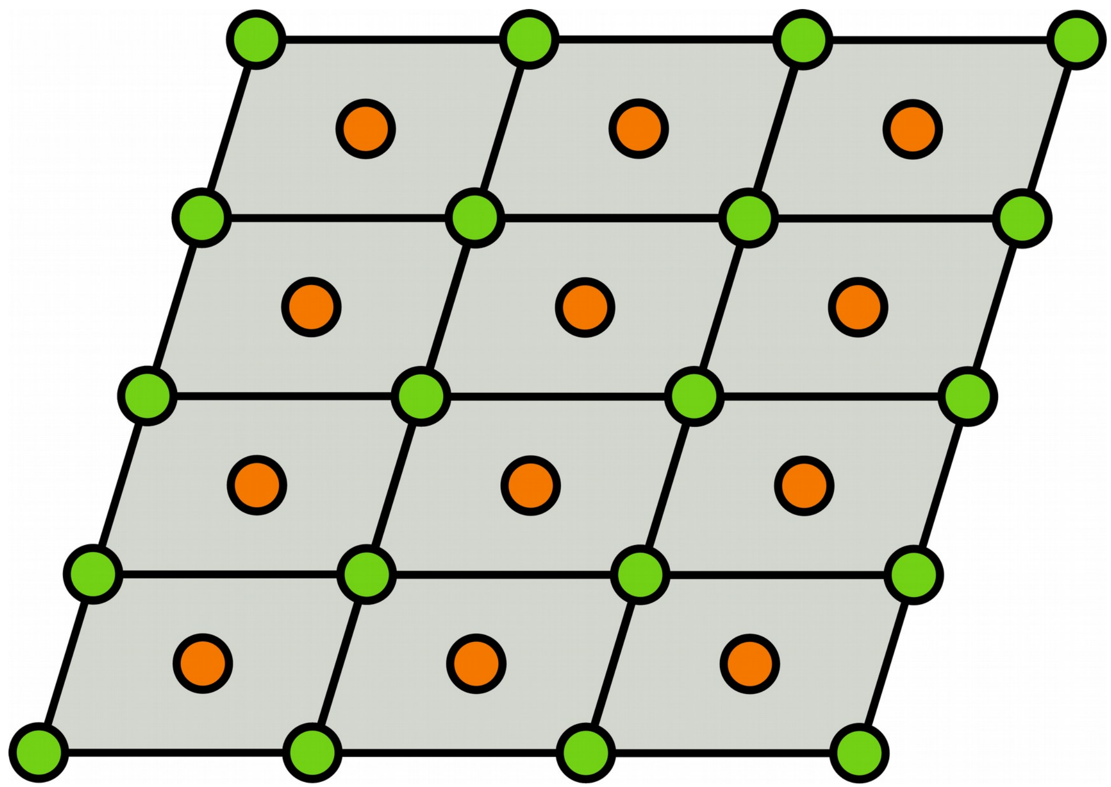
Quasicrystals

Materials 286G
John Goiri

Symmetry

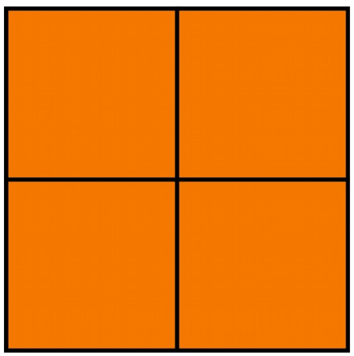
- Only 1, 2, 3, 4 and 6-fold symmetries are possible
- Translational symmetry

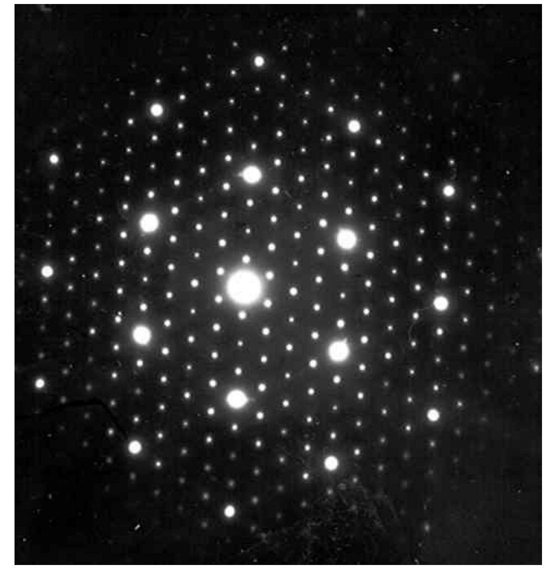


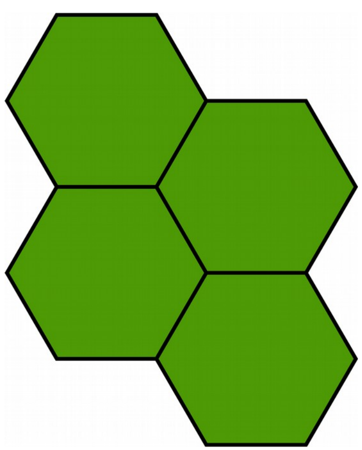


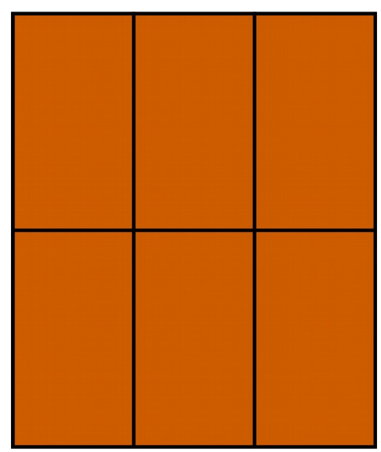
Symmetry

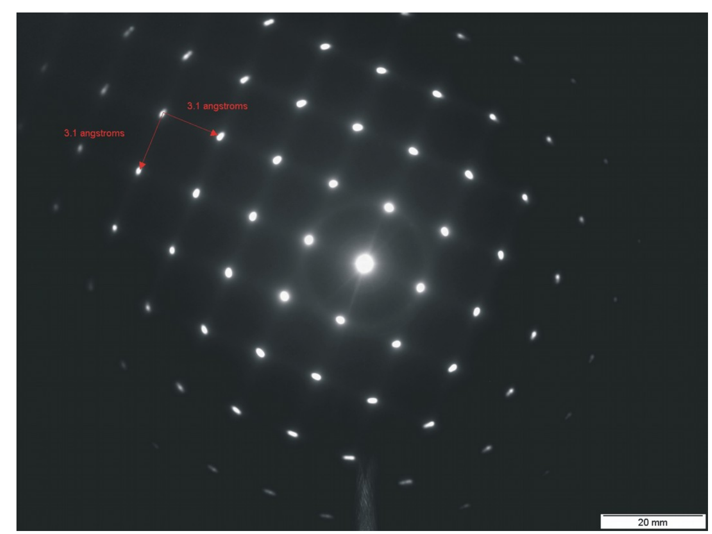
- Allowed symmetries:







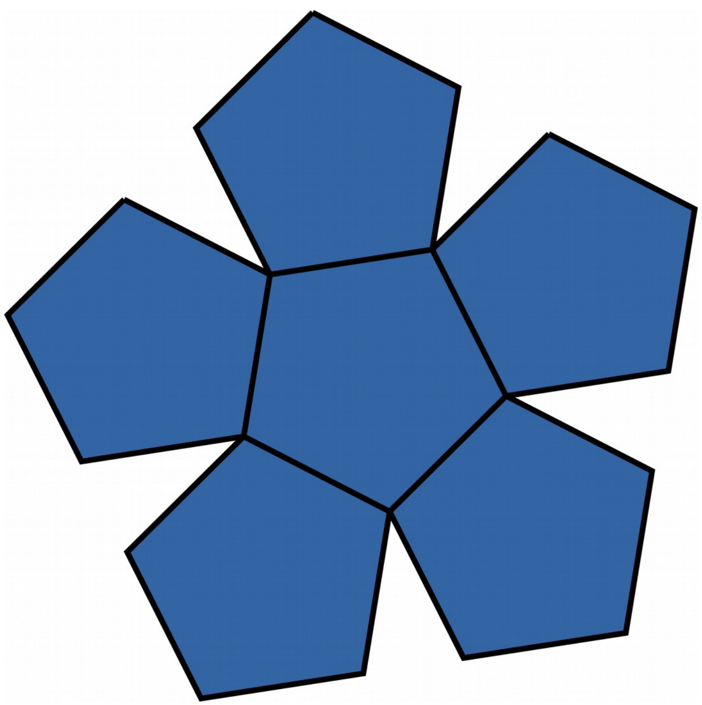


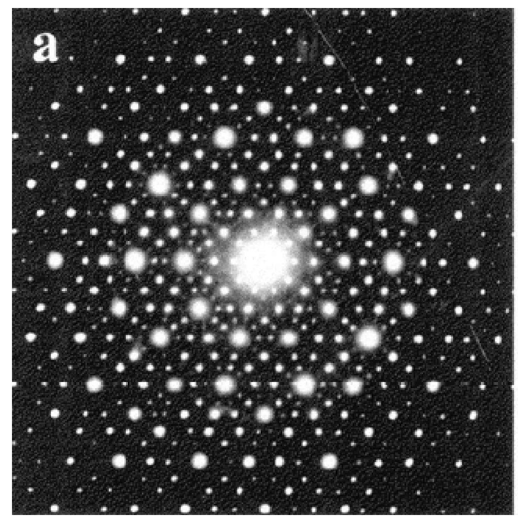


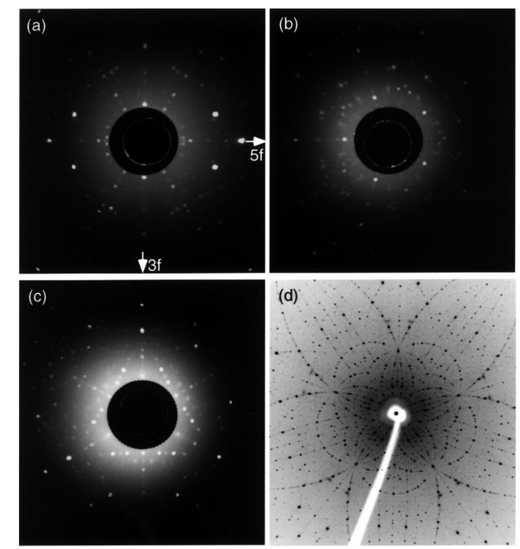
Steinhardt, Paul J, and Luca Bindi. “In Search of Natural Quasicrystals.” Reports on Progress in Physics 75, no. 9 (September 1, 2012): 92601. doi:10.1088/0034-4885/75/9/092601.

Symmetry

- Forbidden symmetries:
- Can't tile space, but X-ray analysis suggests ordering



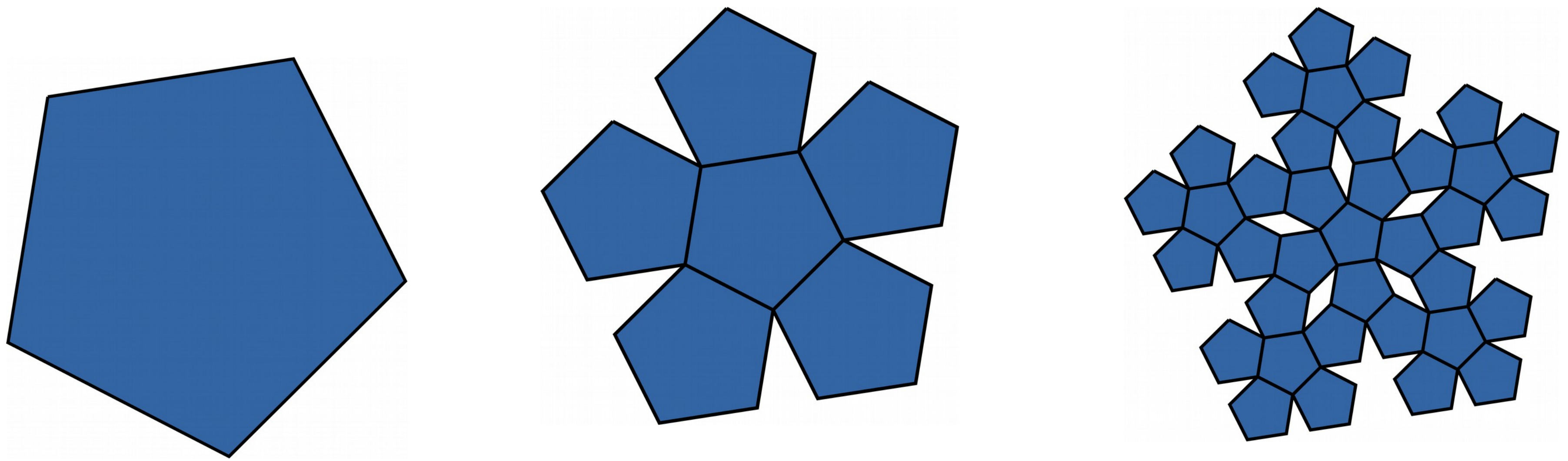




Steinhardt, Paul J, and Luca Bindi. “In Search of Natural Quasicrystals.” Reports on Progress in Physics 75, no. 9 (September 1, 2012): 92601. doi:10.1088/0034-4885/75/9/092601.

Symmetry

- Crystals with forbidden symmetry must have some sort of periodicity
- Can't be translational symmetry
- New kind of symmetry: inflation (recursive)

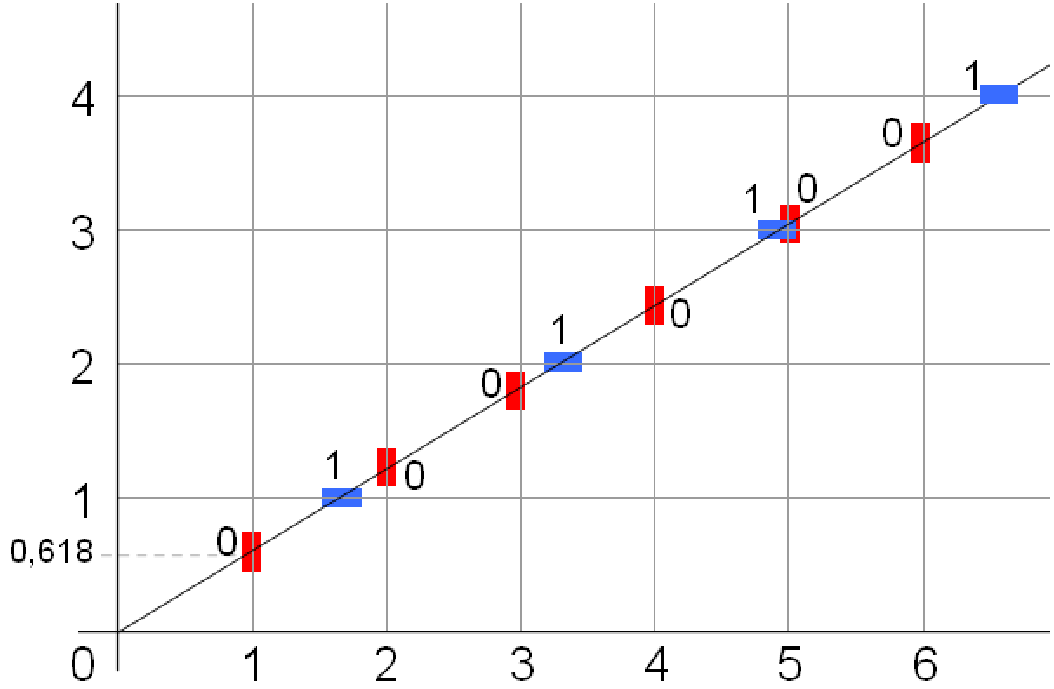


Inflation

- Constructing a Fibonacci word:

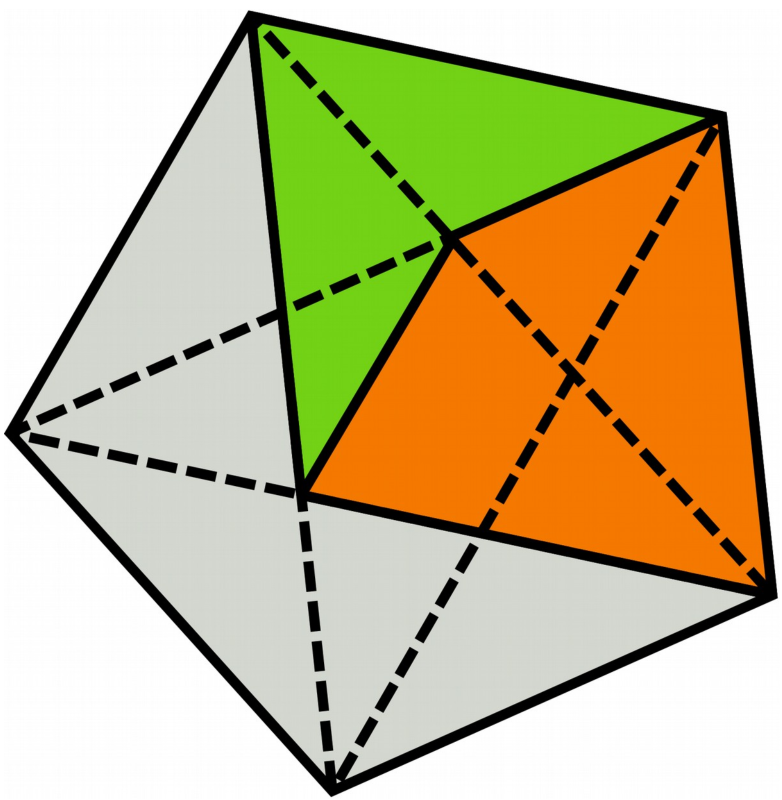
$$S_n = S_{n-1} S_{n-2}$$

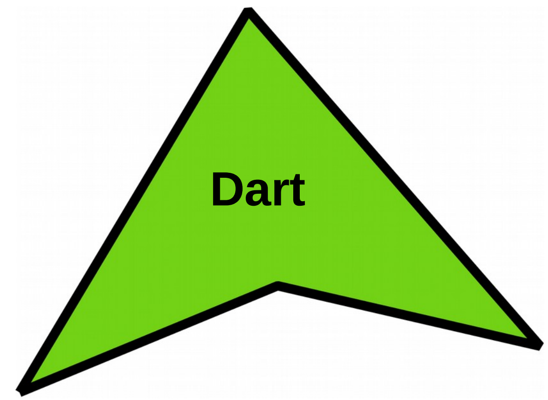
$$\mathrm{S}_0 = 0$$
$$S_1 = 01$$
$$S_2 = 010$$
$$S_3 = 01001$$
$$S_4 = 01001010$$
$$S_5 = 0100101001001$$
$$S_6 = 010010100100101001010$$

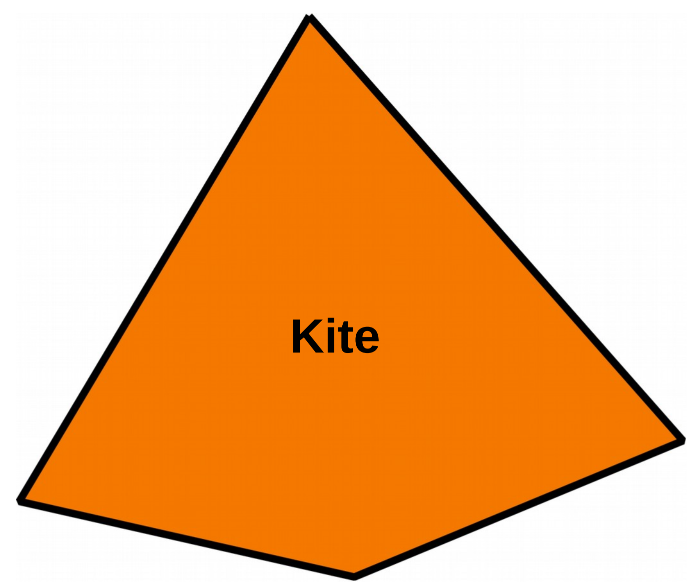


Inflation

- We can inflate 2D shapes to form semiperiodic arrangements
- Also based on golden ratio

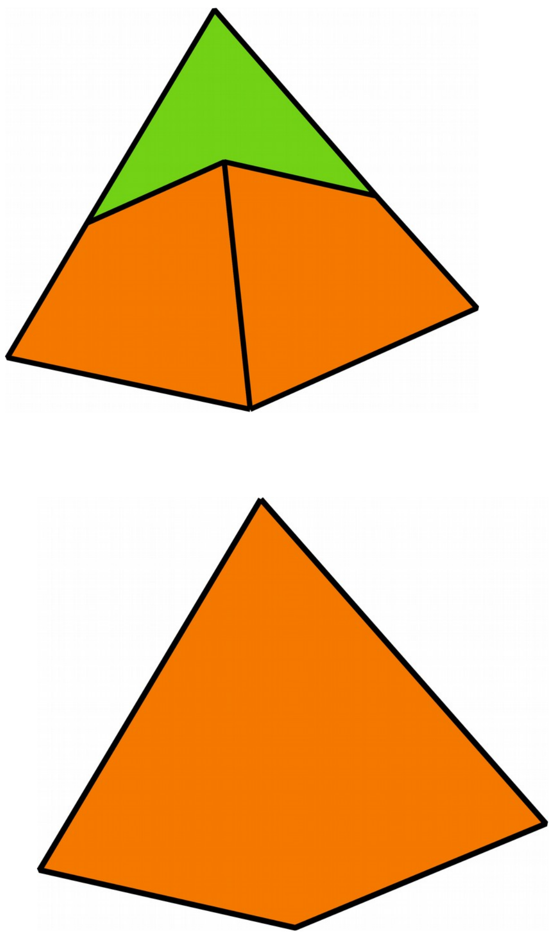


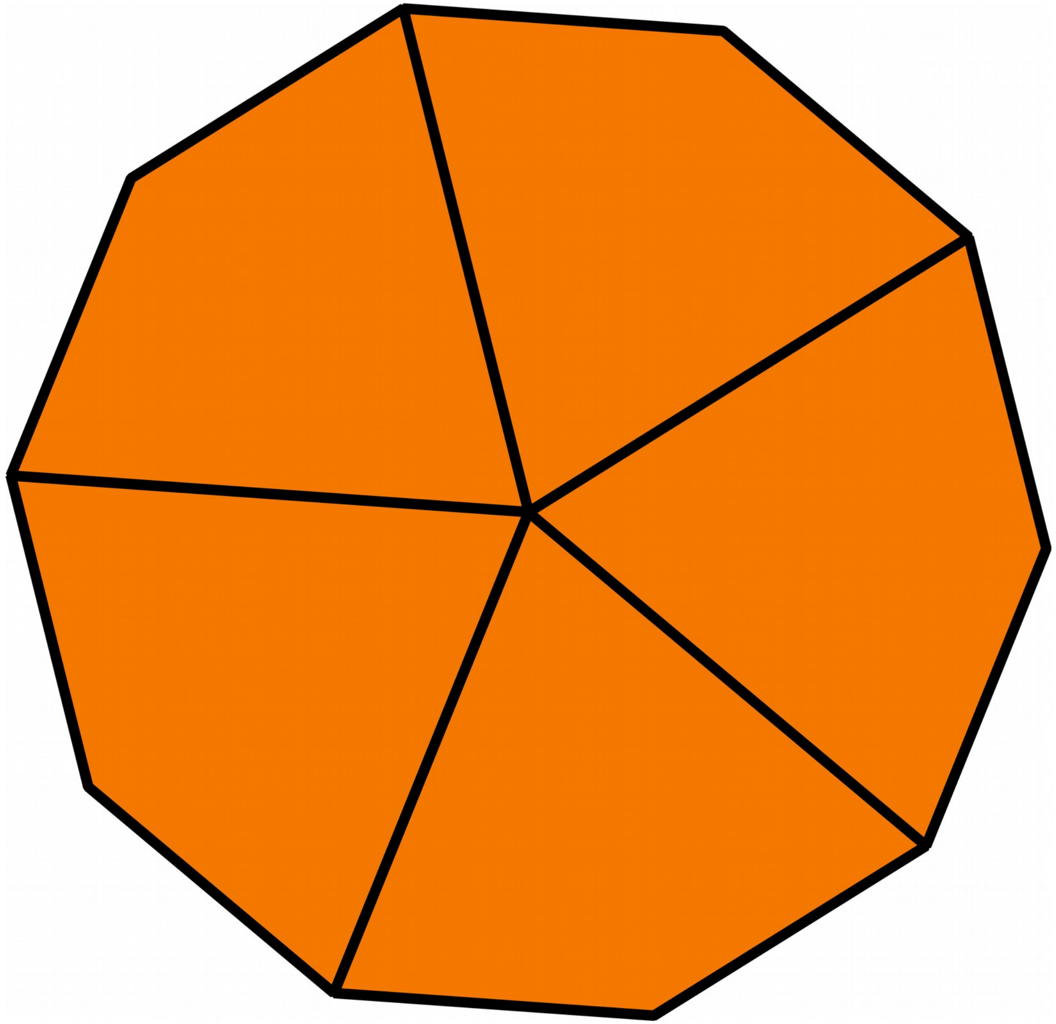




Inflation

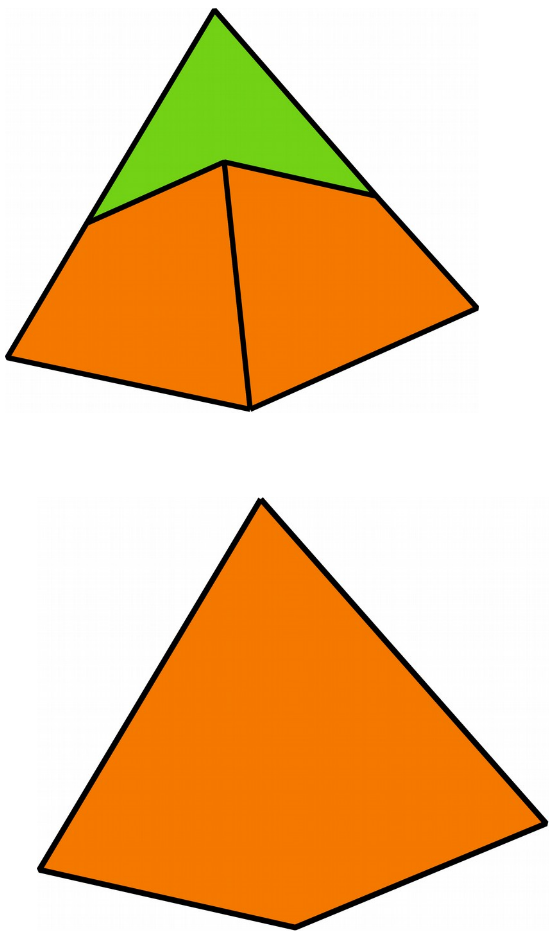
- We can inflate 2D shapes to form semiperiodic arrangements

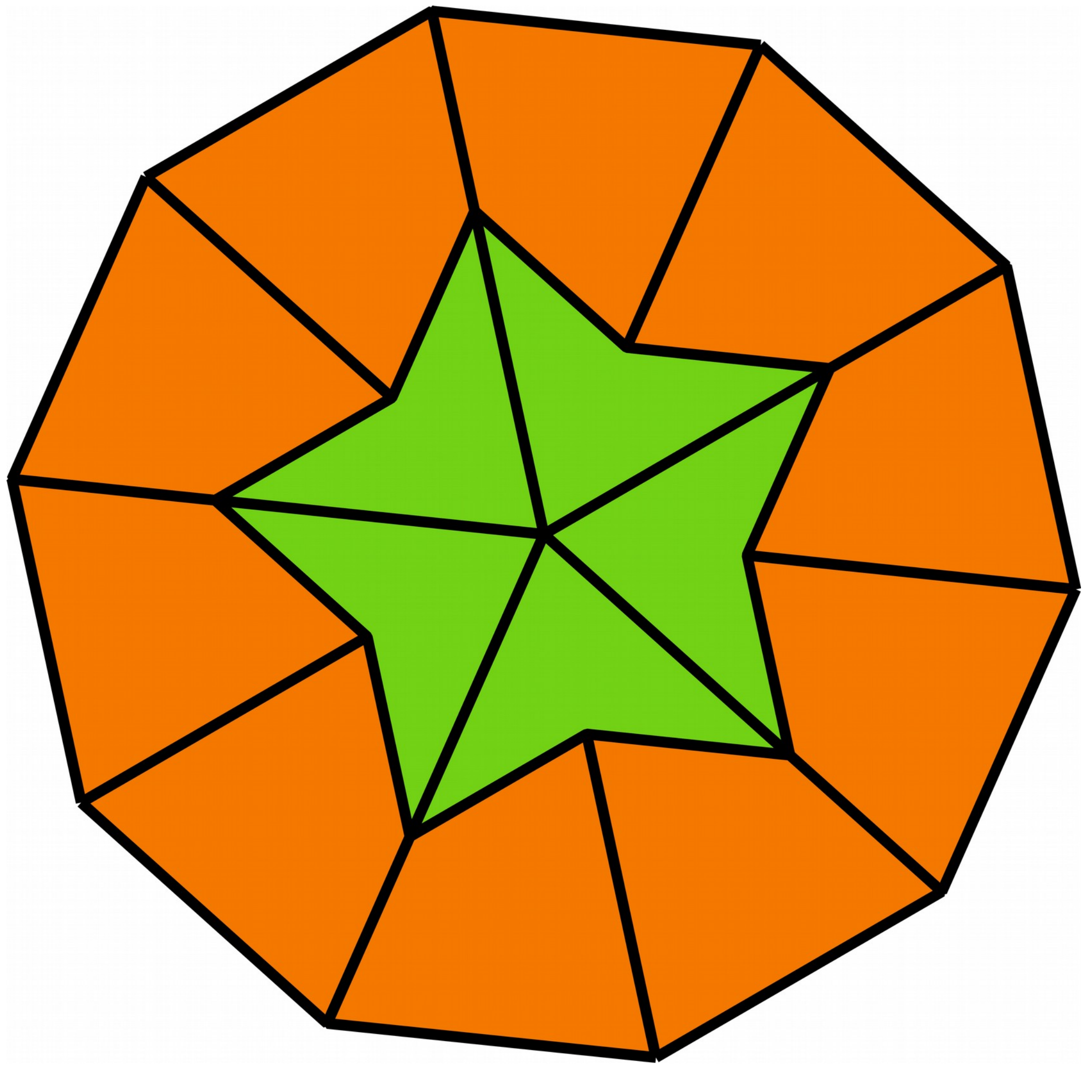




Inflation

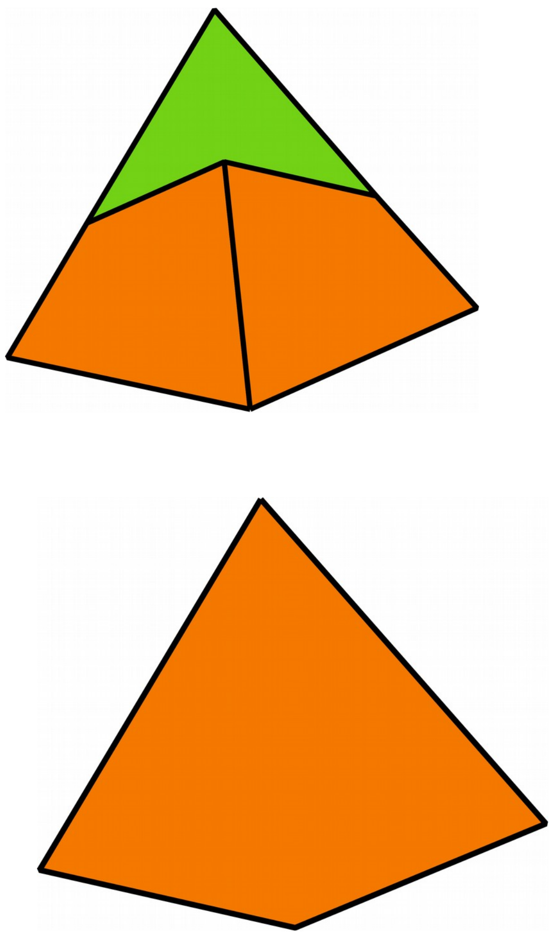
- We can inflate 2D shapes to form semiperiodic arrangements

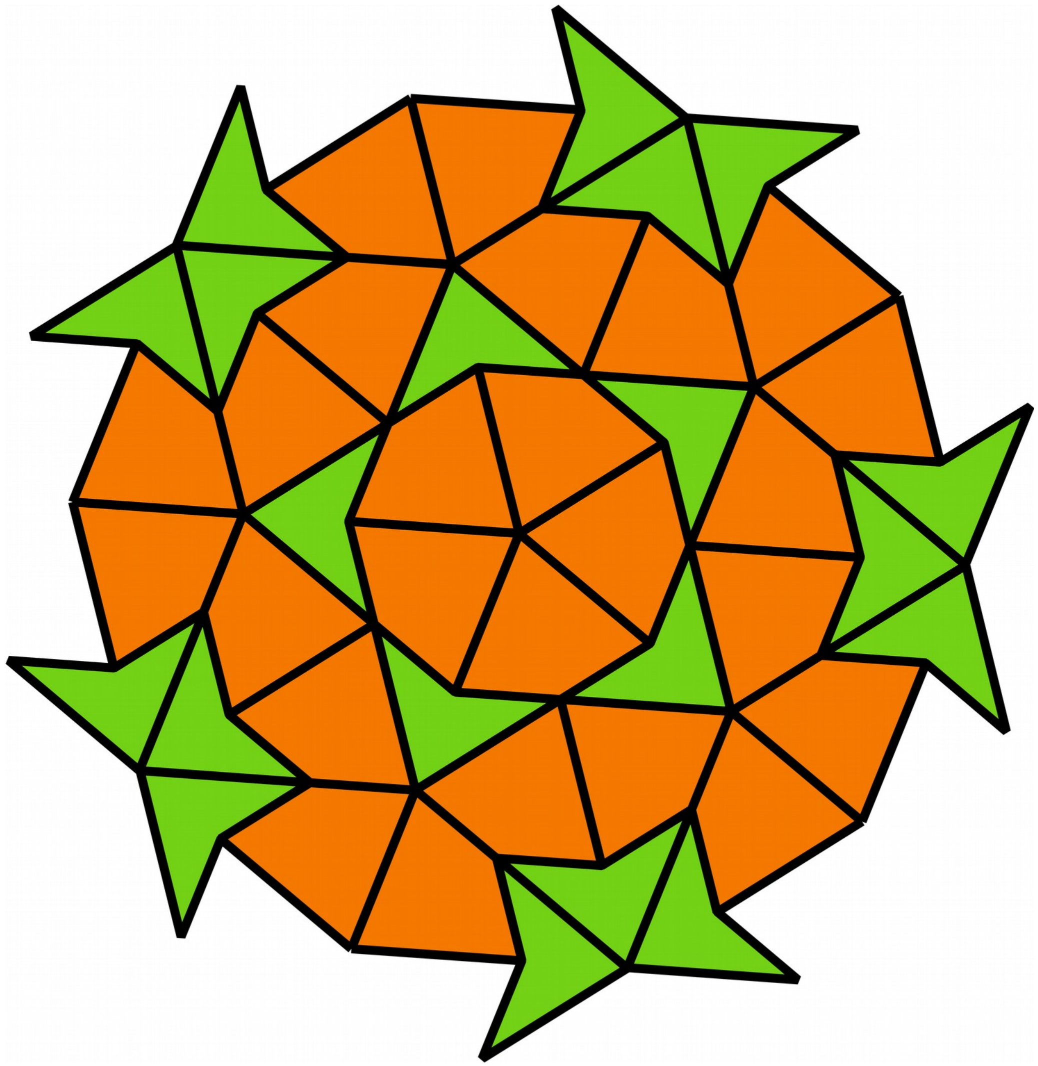




Inflation

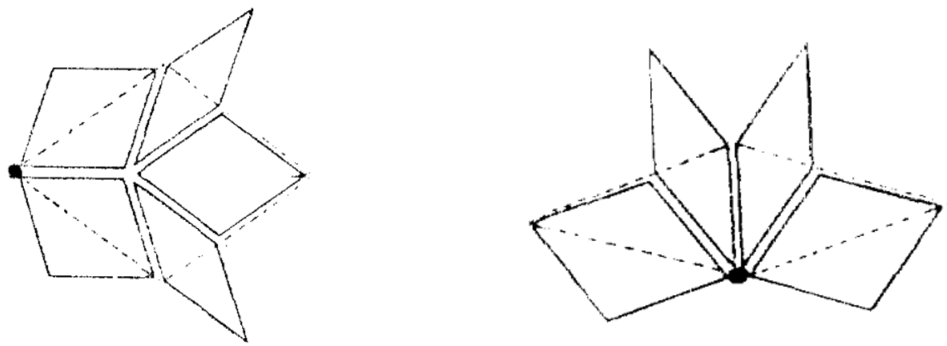
- We can inflate 2D shapes to form semiperiodic arrangements

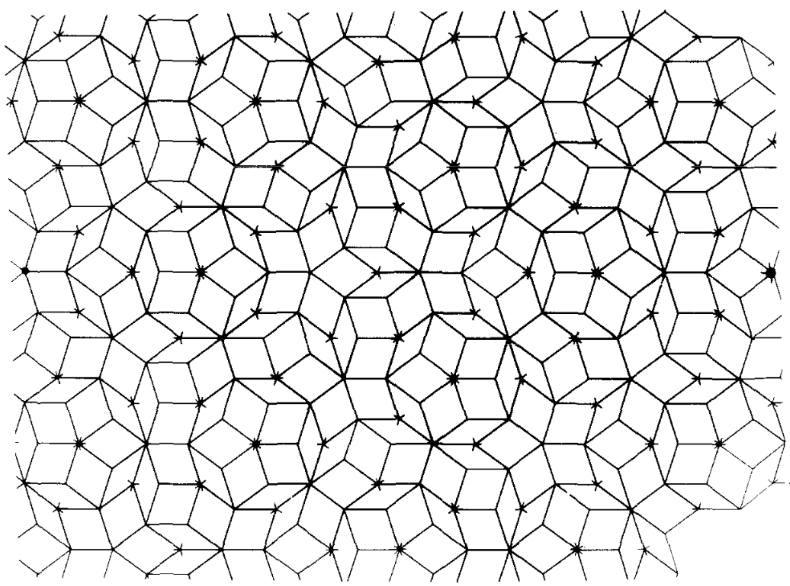


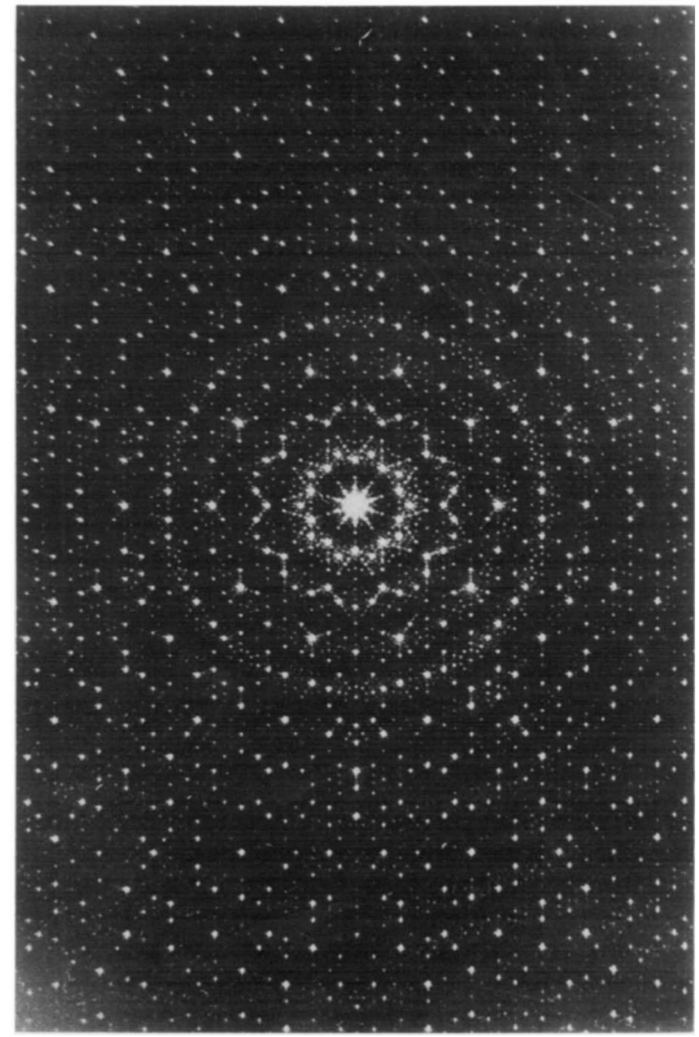


Inflation

- Fourier transform of Penrose tiling reveals a crystalline ordering



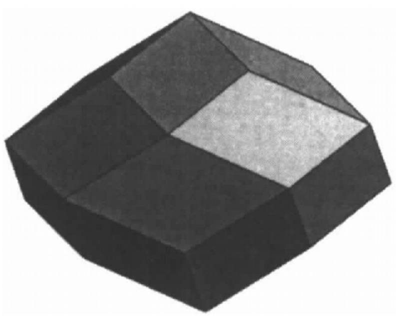


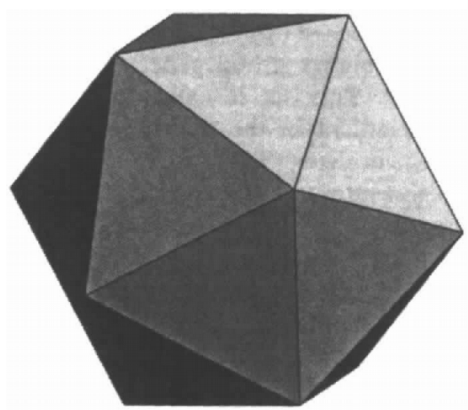


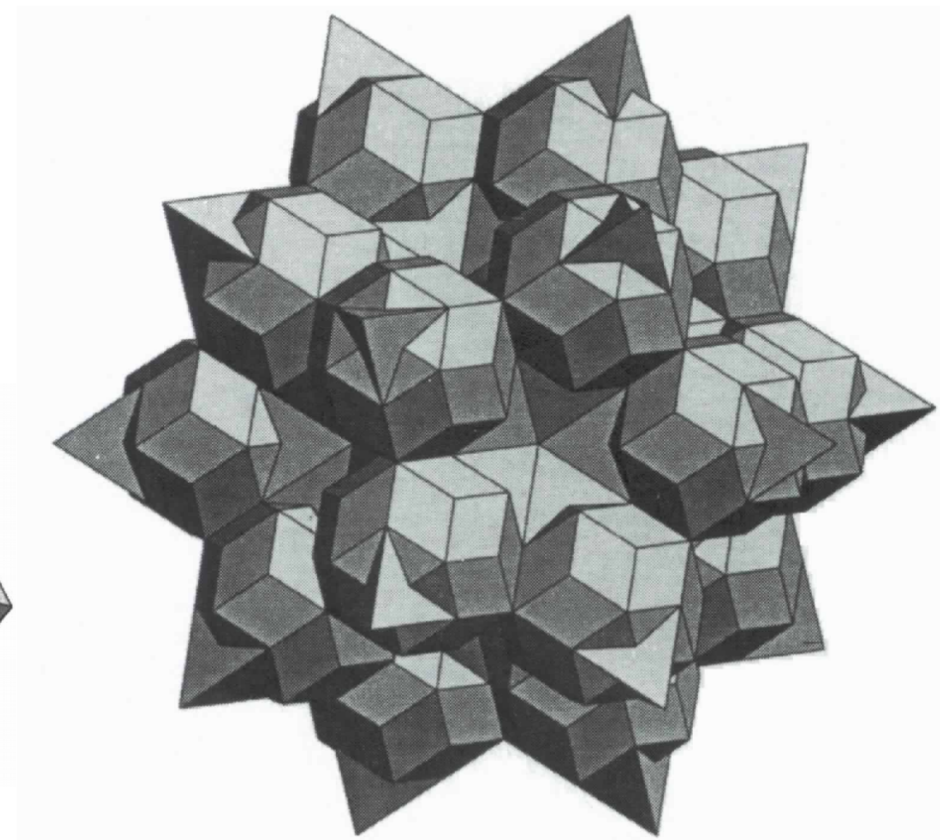
Mackay, Alan L. “Crystallography and the Penrose Pattern.” Physica A: Statistical Mechanics and Its Applications 114, no. 1 (1982): 609–613.

Inflation

- Tiling becomes more complex in 3 dimensional space, but the same principles apply



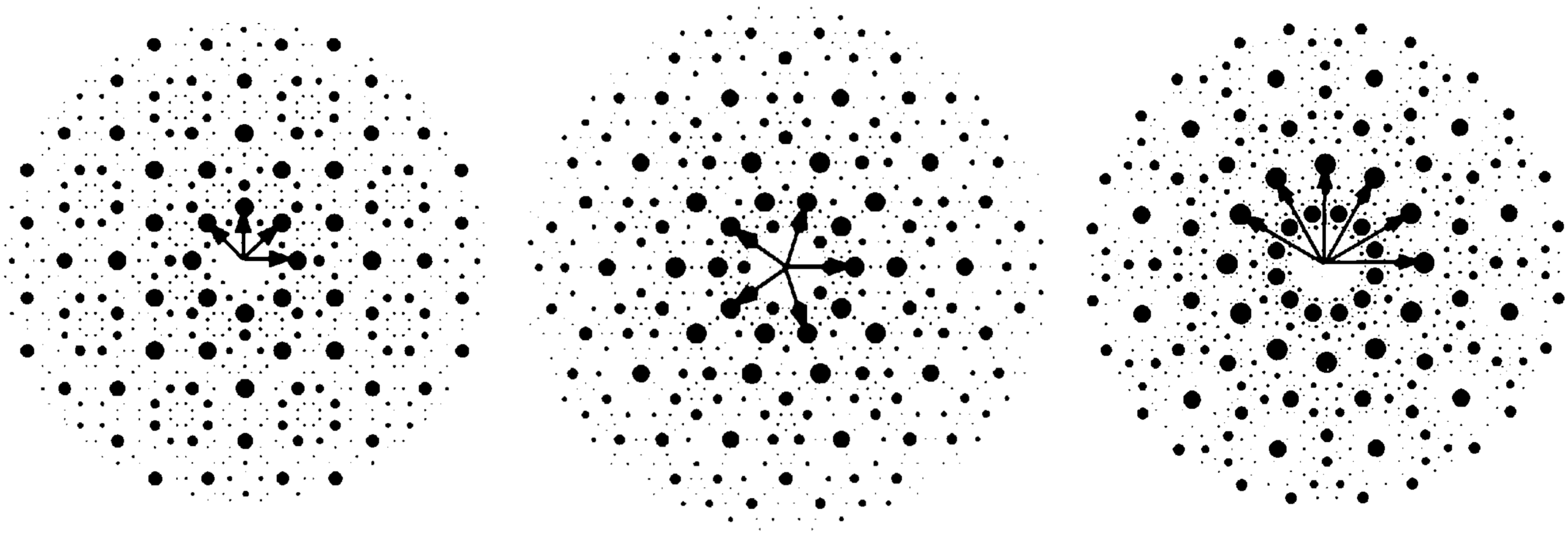




Yamamoto, Akiji. “Crystallography of Quasiperiodic Crystals.” *Acta Crystallographica Section A: Foundations of Crystallography* 52, no. 4 (1996): 509–560.

Quasicrystals as projections

- Diffraction patterns can be thought of as projections from a high dimensional reciprocal lattice onto 2 dimensions



Yamamoto, Akiji. “Crystallography of Quasiperiodic Crystals.” *Acta Crystallographica Section A: Foundations of Crystallography* 52, no. 4 (1996): 509–560.

Quasicrystals as projections

- High dimensional projections can be visualized by simplifying down to a 1 dimensional crystal
- As intersection becomes irrational, projection becomes non-periodic

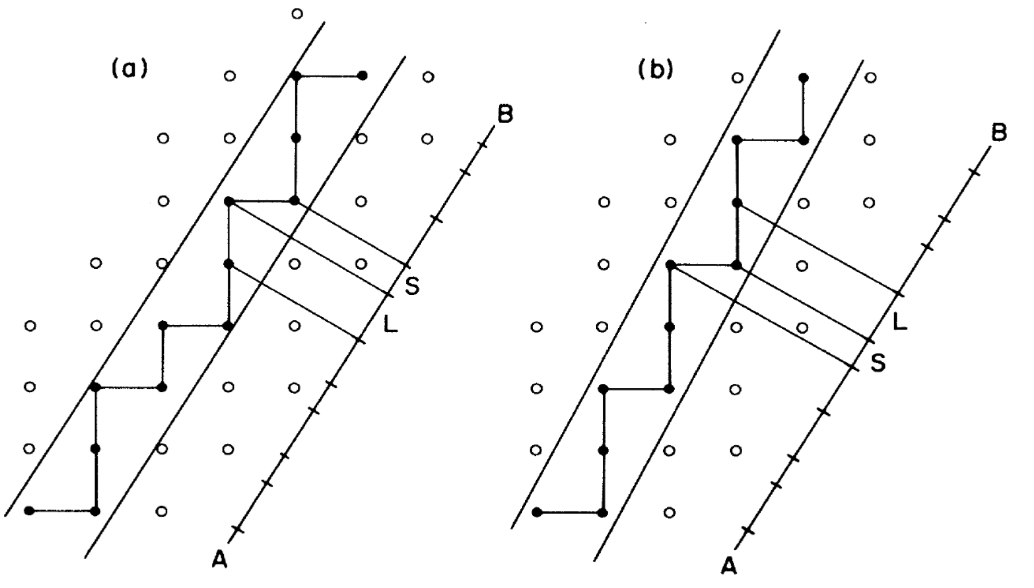


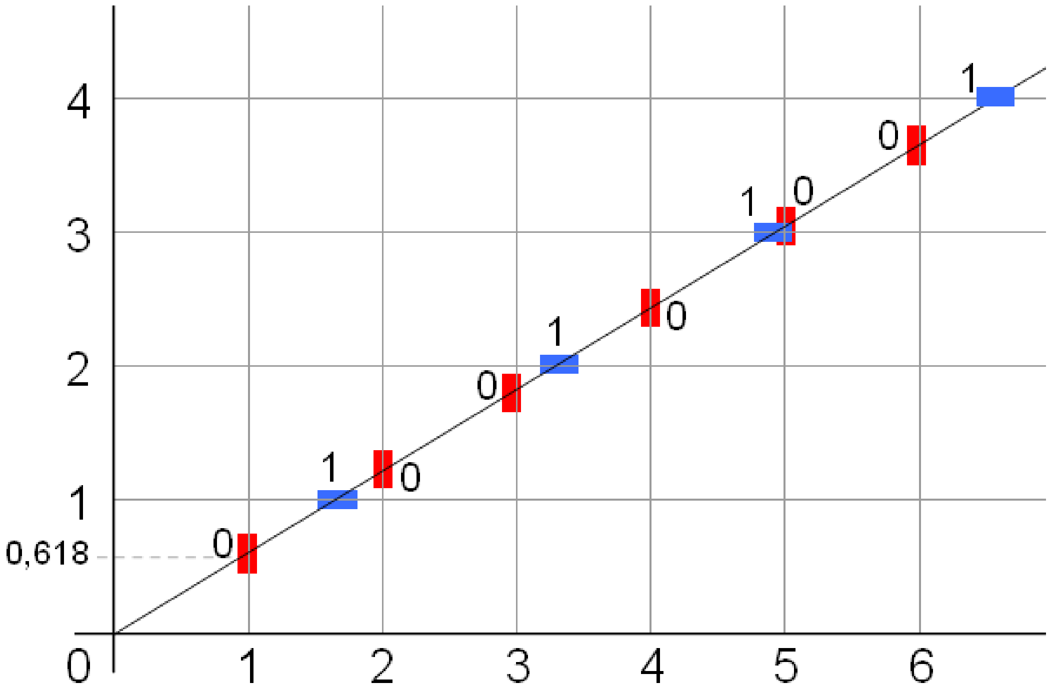
FIG. 1. (a) Incommensurate strip generating quasiperiodic tiling; (b) commensurate strip generating periodic tiling.

Yamamoto, Akiji. “Crystallography of Quasiperiodic Crystals.” *Acta Crystallographica Section A: Foundations of Crystallography* 52, no. 4 (1996): 509–560.

Quasicrystals as projections

- Quasicrystal unit cell can be approximated by approximating the intersection
- Approximating a Fibonacci word:

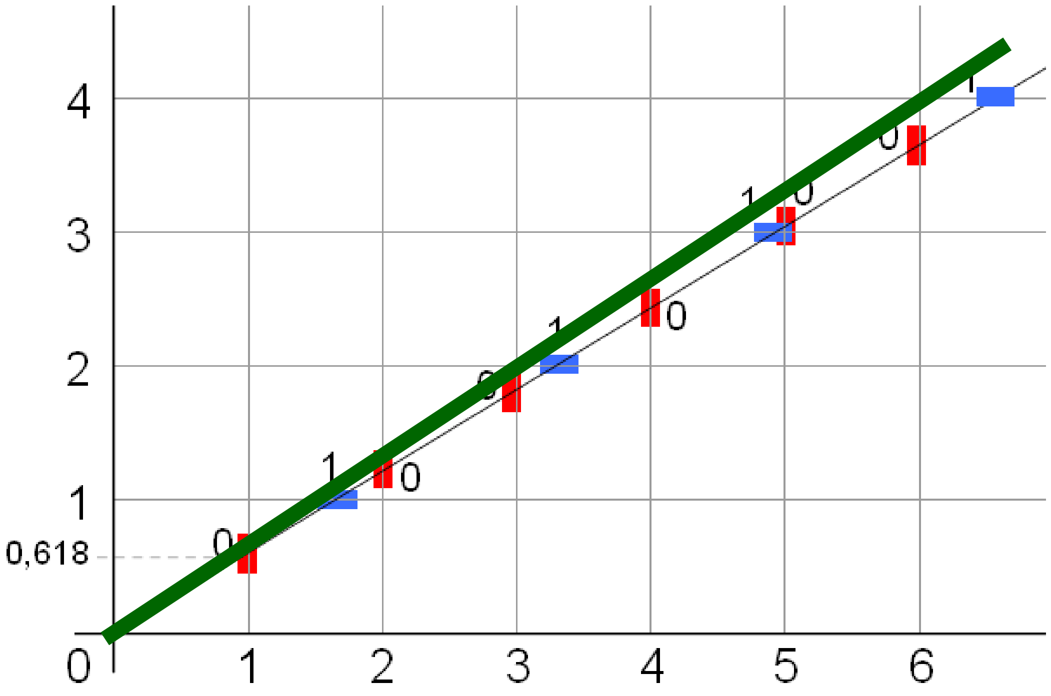
$$S_0 = 0$$
$$S_1 = 01$$
$$S_2 = 010$$
$$\dots$$
$$S_n = 0100101001001\dots$$



Quasicrystals as projections

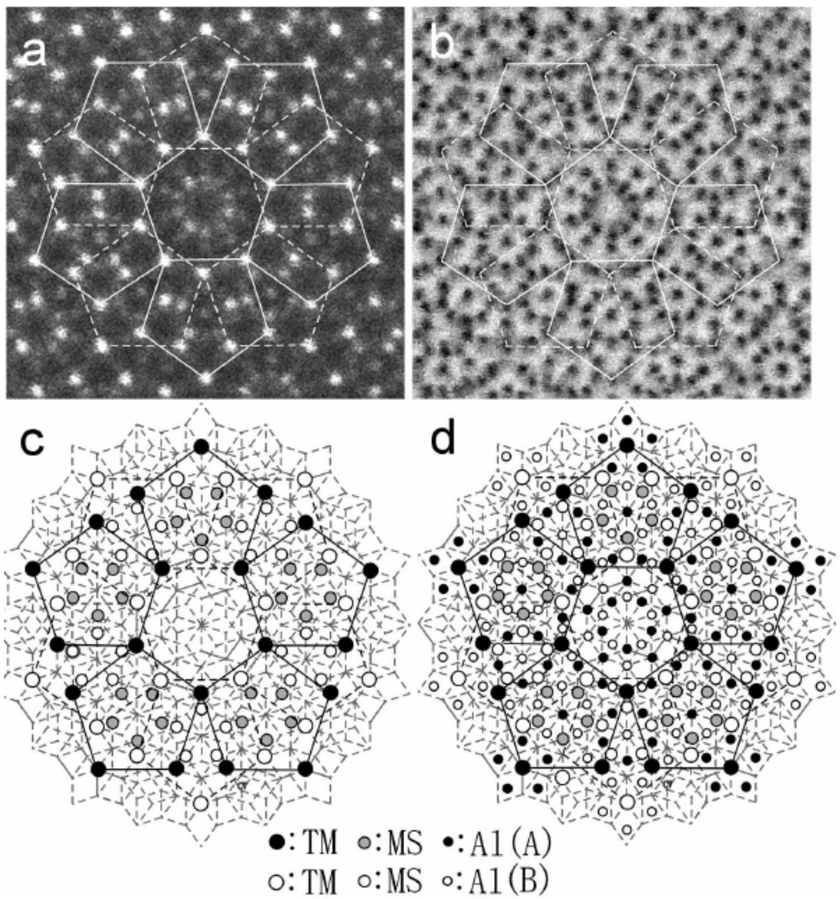
- Quasicrystal unit cell can be approximated by approximating the intersection
- Approximating a Fibonacci word:

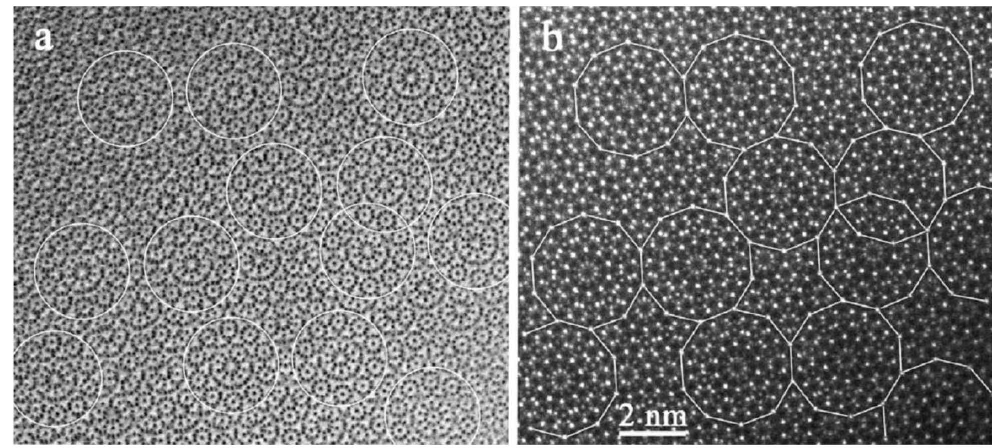
$$
\begin{aligned}
S_0 &= 0 \\
S_1 &= 01 \\
S_2 &= 010 \\
&\ldots \\
S_n &= 0100101001001\ldots \\
&\approx 01001001001001\ldots
\end{aligned}
$$



Known quasicrystals

- $Al_{72}Ni_{24}Fe_4$ (found in a meteorite!)

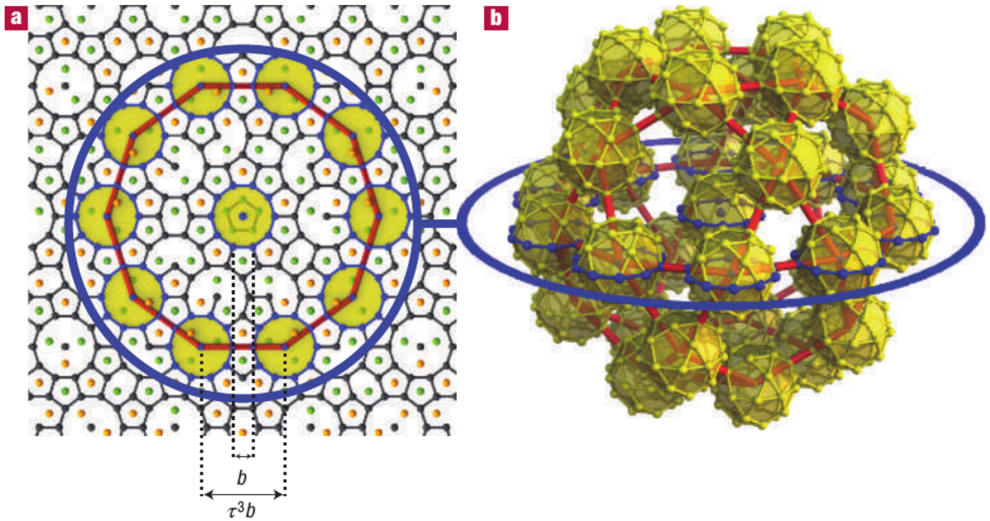


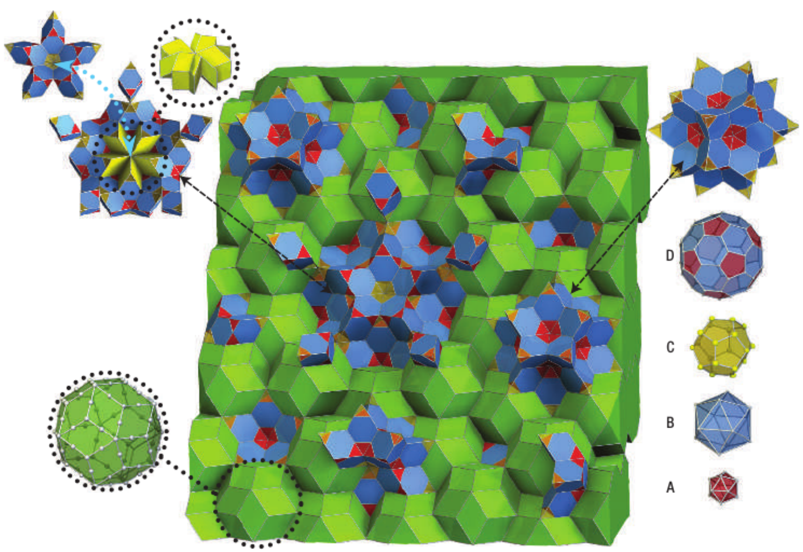


Yasuhara, A., K. Yamamoto, K. Yubuta, and K. Hiraga. “Structure of an Al-Fe-Ni Decagonal Quasicrystal Studied by Cs-Corrected STEM.” *Acta Physica Polonica A* 126, no. 2 (August 2014): 637–40. doi:10.12693/APhysPolA.126.637.

Known quasicrystals

- Yb-Cd





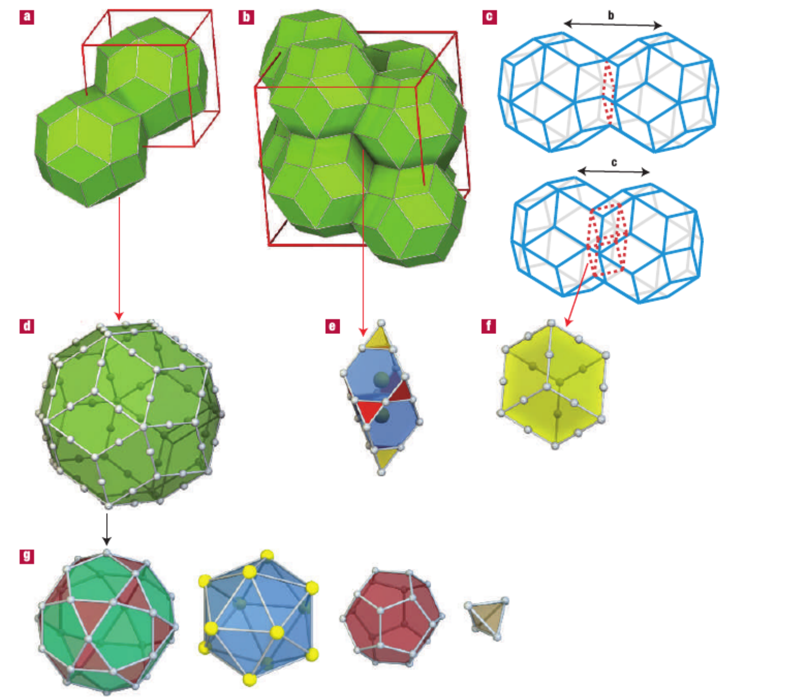
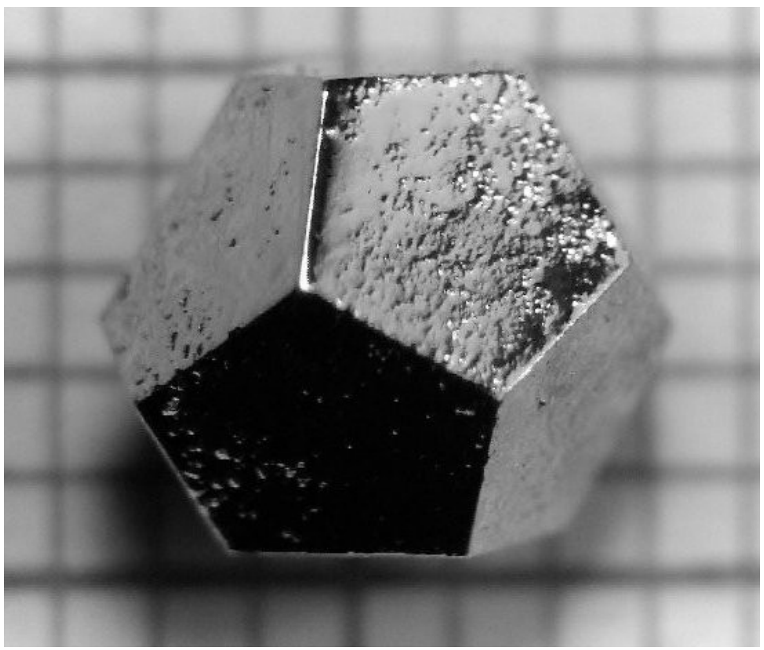


Figure 1 Approximants, building units and linkages. a, The body-centred-cubic packing of RTH units in the 1/1 cubic approximant. **b**, The packing of RTH units in the 2/1 cubic approximant. **c**, The two different types of linkages between the RTH units. The **b**- and **c**-linkage occurs along the two- and three-fold directions, respectively. **d–f**, The three fundamental building units: RTH (**d**), AR (**e**) and OR (**f**), and their corresponding atomic decorations. All rhombic faces of these three building units are decorated with Cd atoms on the vertices and mid-edges. **g**, Atomic sub-shells inside the RTH unit (92 atoms, $R = 0.78$ nm along its two-fold direction). From left to right: a Cd icosidodecahedron (30 atoms, $R = 0.65$ nm), a Yb icosahedron (12 atoms, $R = 0.56$ nm), a Cd dodecahedron (20 atoms, $R = 0.46$ nm), and the inner Cd tetrahedron (4 atoms, occurring in different orientations). All Cd atoms are shown in grey and Yb atoms in yellow. The red arrows indicate where in the approximant structures the corresponding building units can be found.

Guo, J.Q., E. Abe, and A.P. Tsai. "A New Stable Icosahedral Quasicrystal in the Cd-Mg-Dy System." *Philosophical Magazine Letters* 81, no. 1 (January 2001): 17–21. doi:10.1080/09500830010008411.

Known quasicrystals

- Al-Co-Ni, Al-Cu-Co, Al-Li-Cu, Al-Pd-Mn...
- Symmetry reflected at macroscopic scale



Ho-Mg-Zn

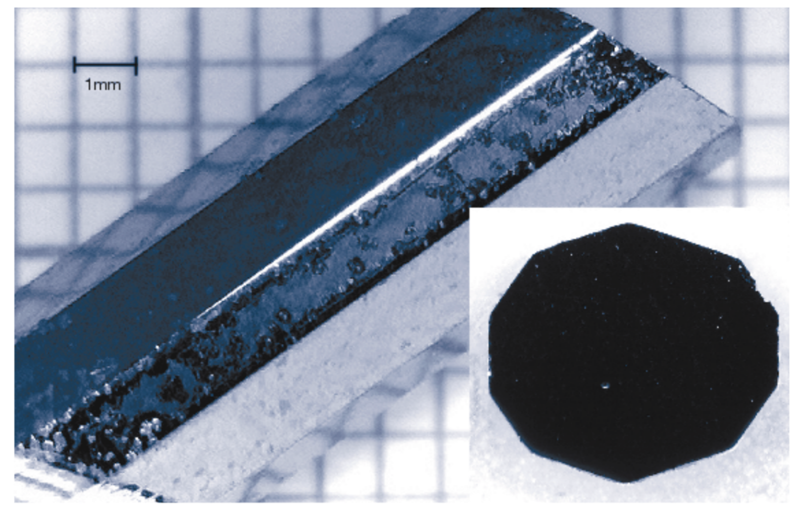


Figure 1 **Quasicrystals show unusual symmetry not seen in normal metallic crystals. A single grain[7] of Al-Ni-Co decagonal quasicrystal shows tenfold symmetry over a millimetre grid. Note reflections of millimetre scale on side facets. Whereas the main figure shows just five of the ten facets clearly, the inset shows a view of a polished surface seen down the tenfold axis with all ten edges visible. The ten facets exposed at the surface reflect the atomic-scale symmetry. Experiments by Rotenberg *et al.*[1]**

Al-Co-Ni

Sato, Taku J., Hiroyuki Takakura, and An Pang Tsai. “Single Crystal Growth of the Icosahedral Zn-Mg-Ho Quasicrystal.” *Japanese Journal of Applied Physics* 37, no. 6A (1998): L663.

Unknown quasicrystals

- Semiperiodic crystals can retain “normal” symmetry
- Fibonacci grid

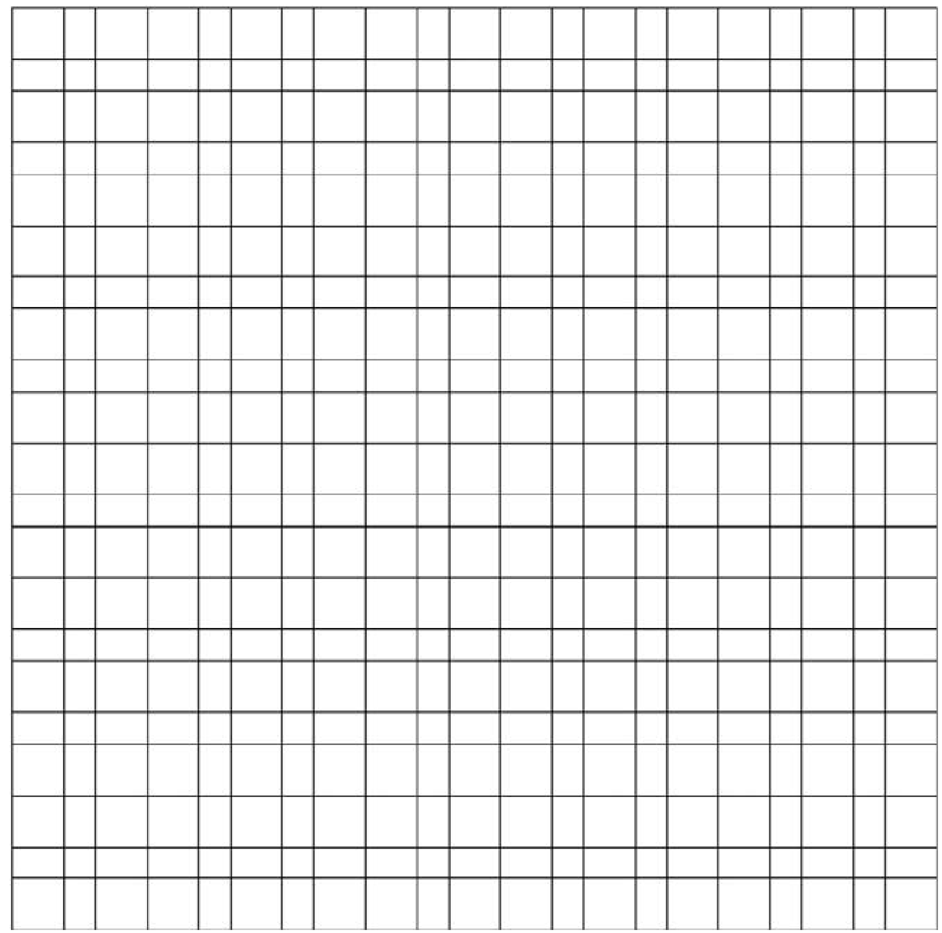
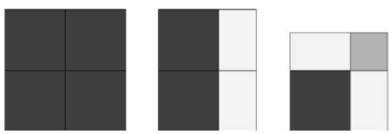


Fig. 1. The square Fibonacci tiling.

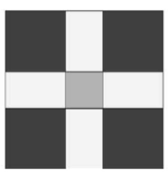
Lifshitz, Ron. “The Square Fibonacci Tiling.” *Journal of Alloys and Compounds* 342, no. 1 (2002): 186–190.

Unknown quasicrystals

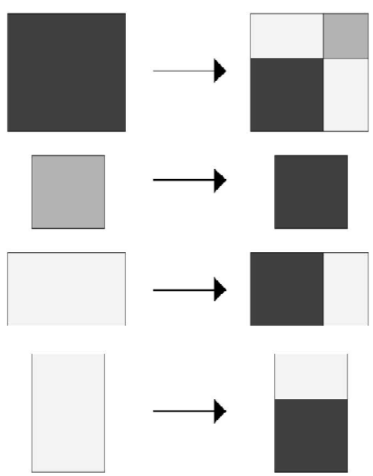
- Has both 4mm symmetry **and** inflation symmetry

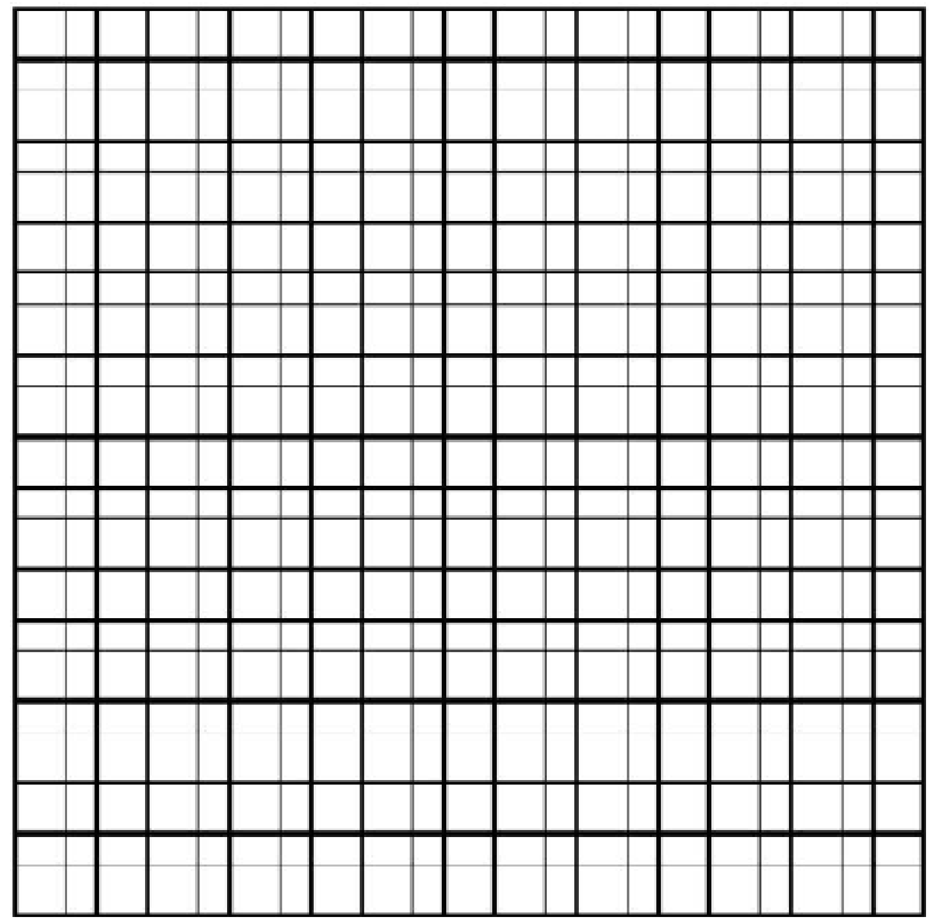


(a)



(b)

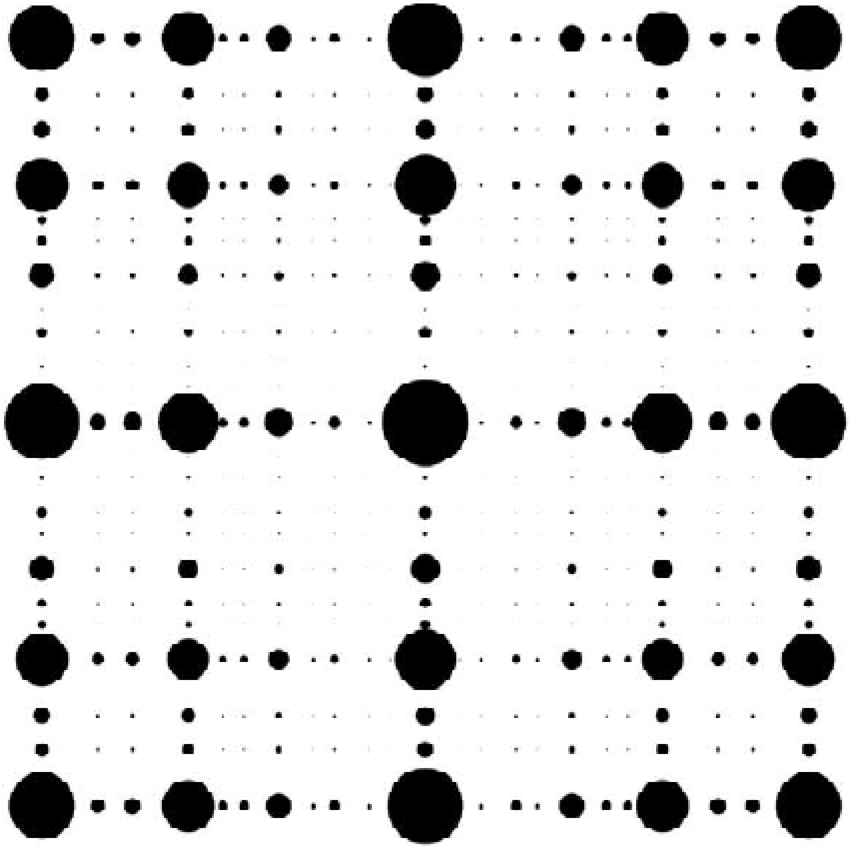




Lifshitz, Ron. “The Square Fibonacci Tiling.” *Journal of Alloys and Compounds* 342, no. 1 (2002): 186–190.

Unknown quasicrystals

- Fourier transform has tetragonal symmetry, but contains fractal like spots
- So far not observed in any material



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