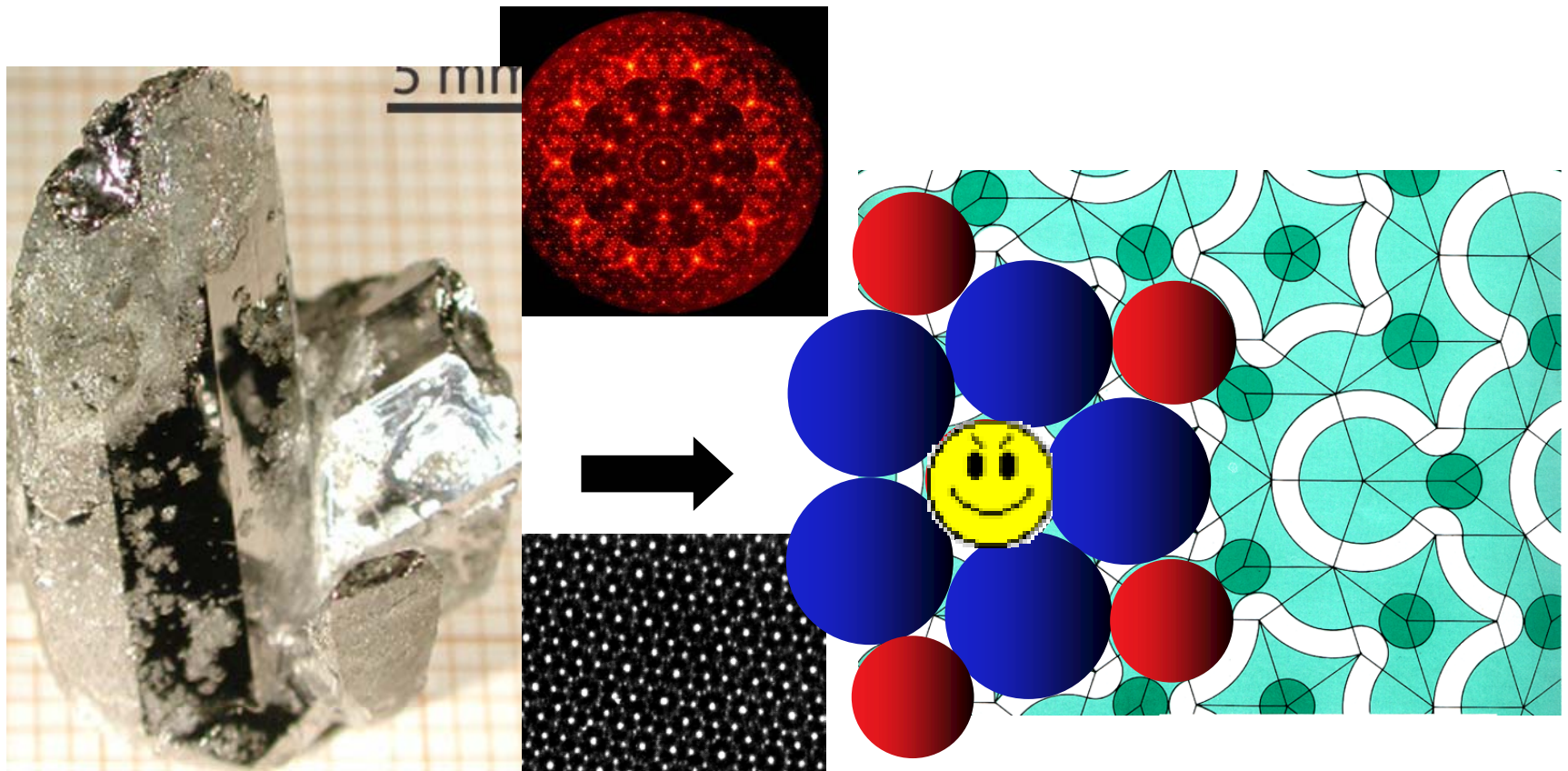
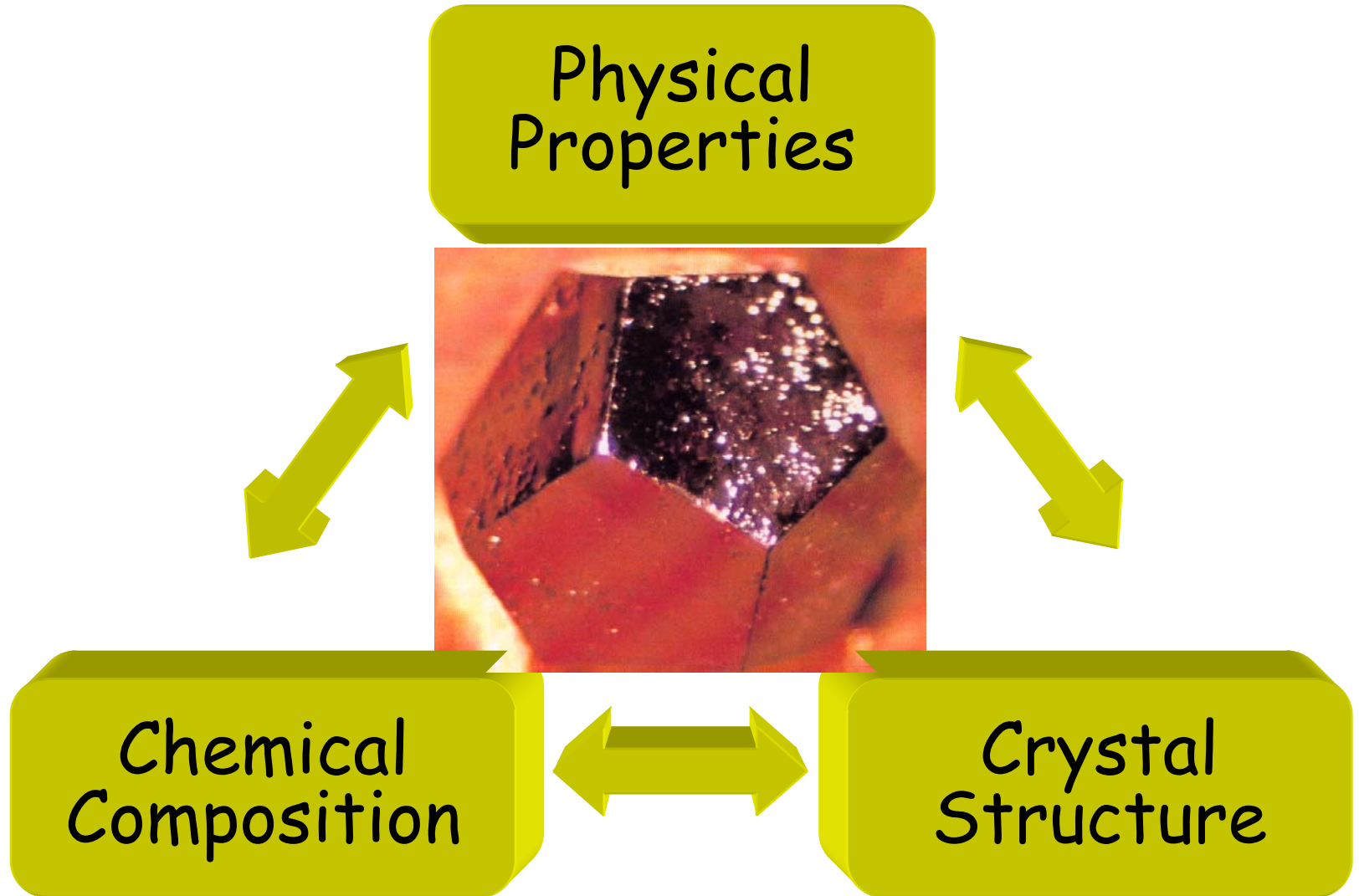


Structural Modelling - Where are the atoms and why?

W. Steurer, A. Cervellino, M. Kobas, T. Weber



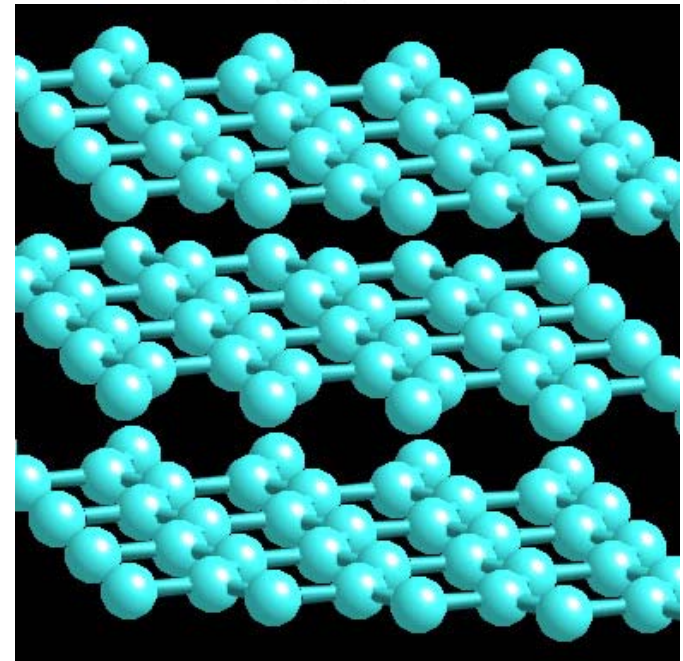
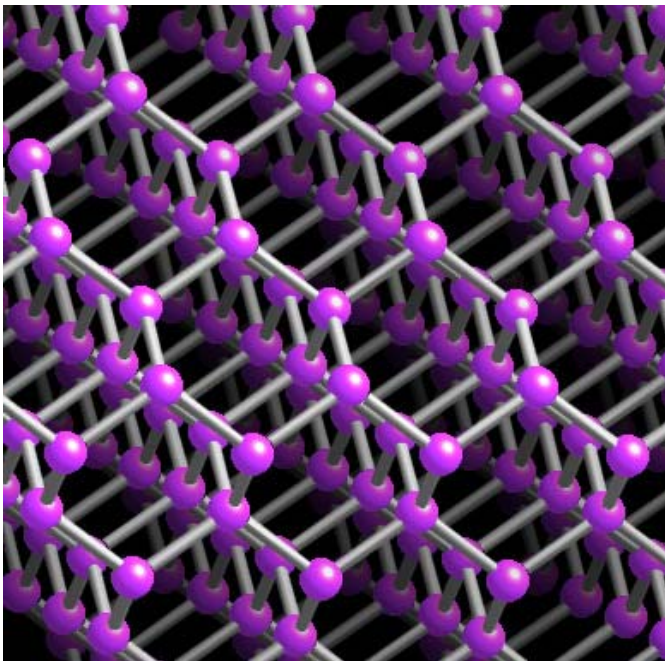
Why are we interested in the crystal structure of a material?



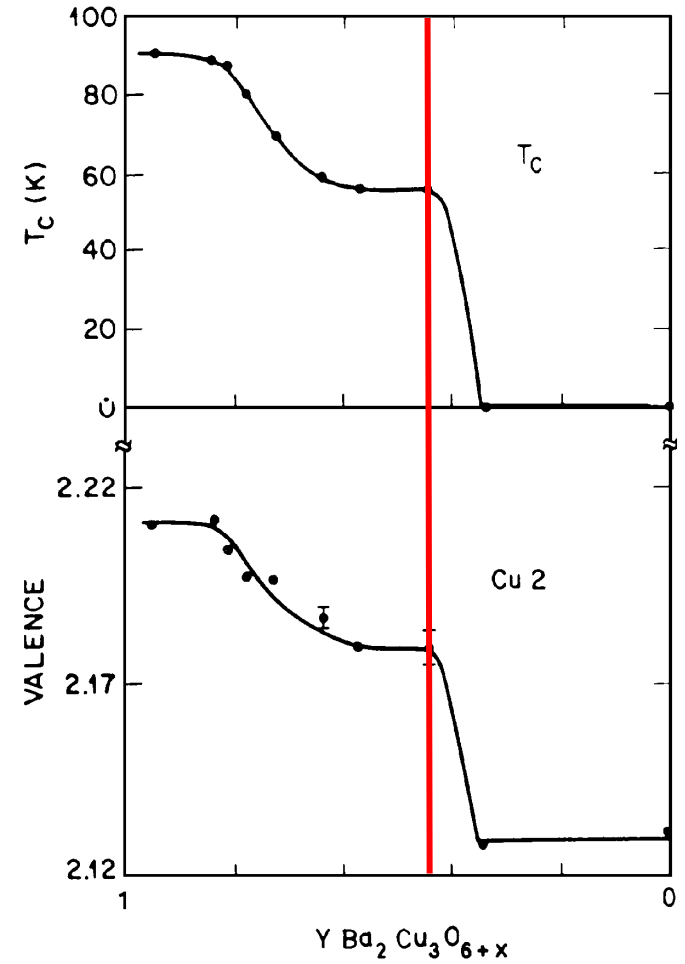
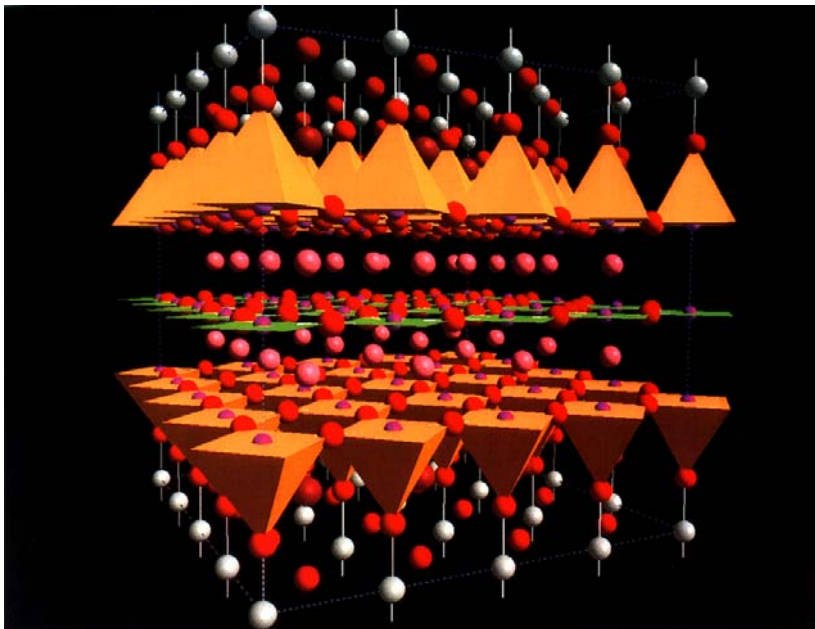
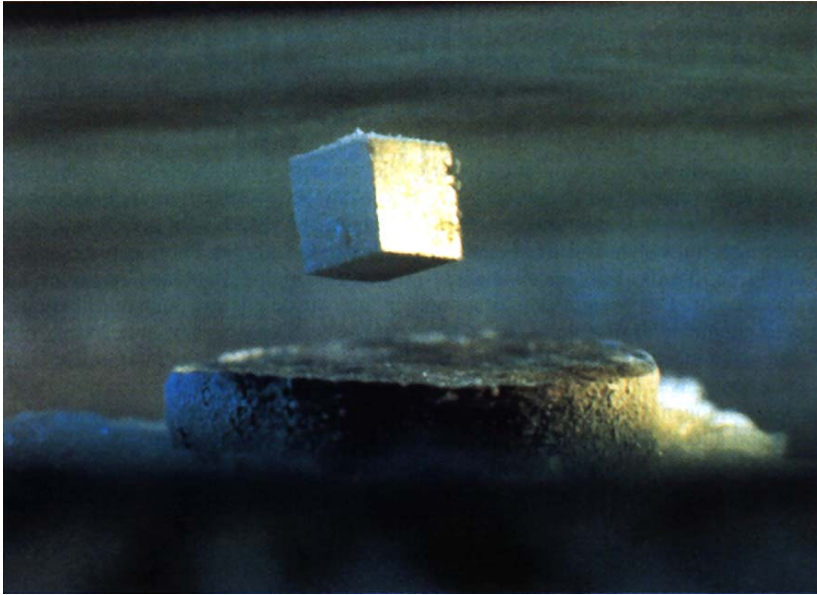
Structure property relationships



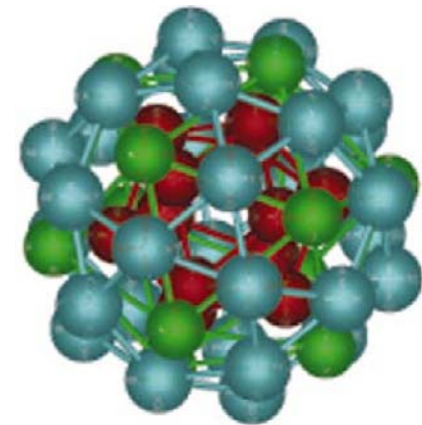
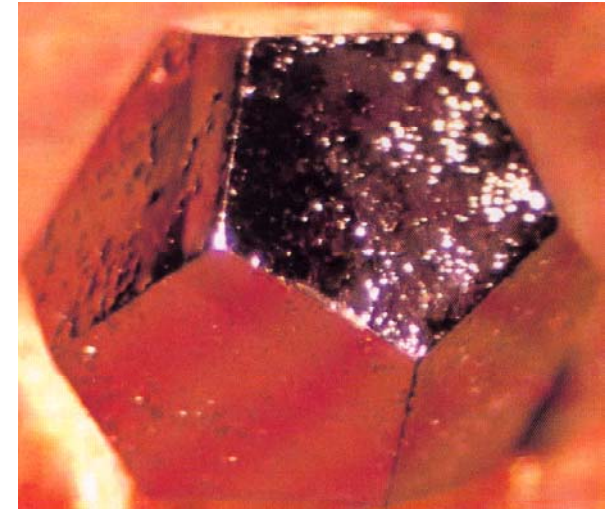
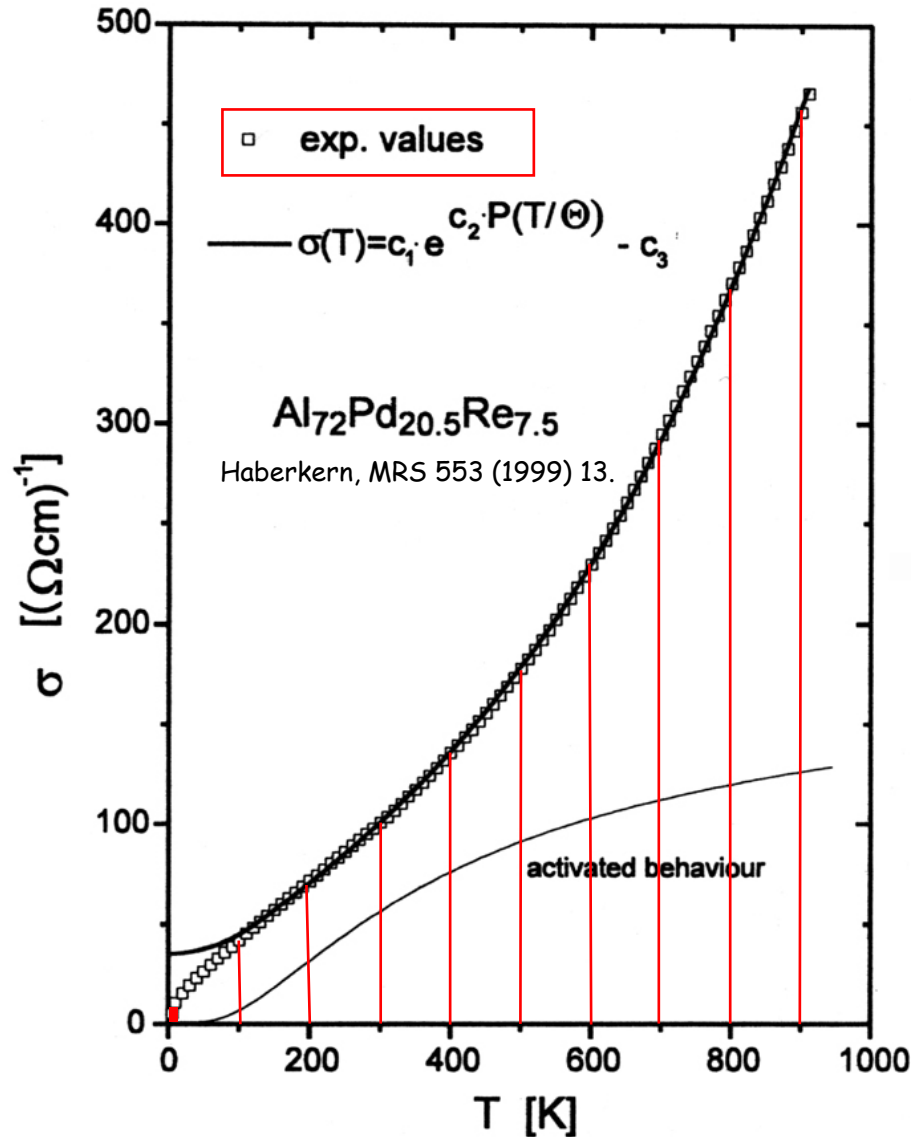
C



Structure property relationships

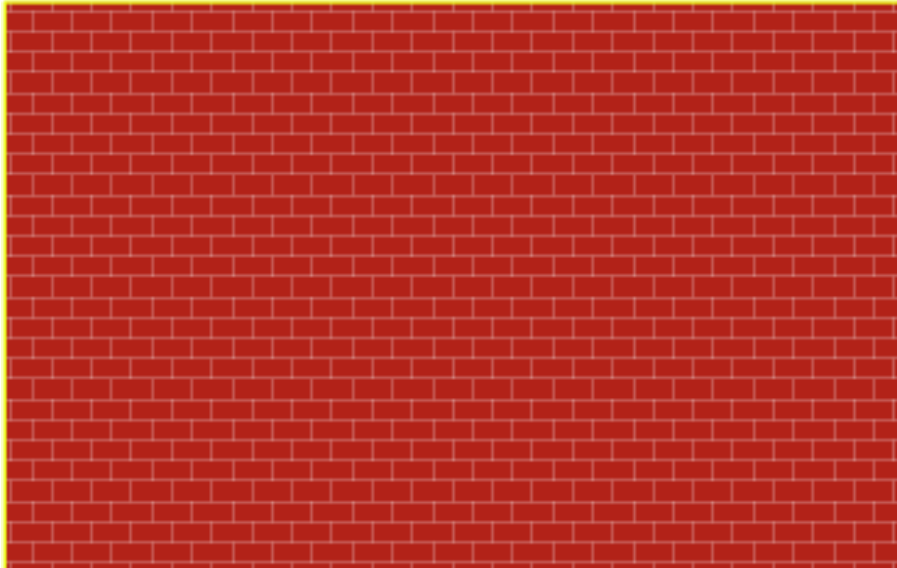
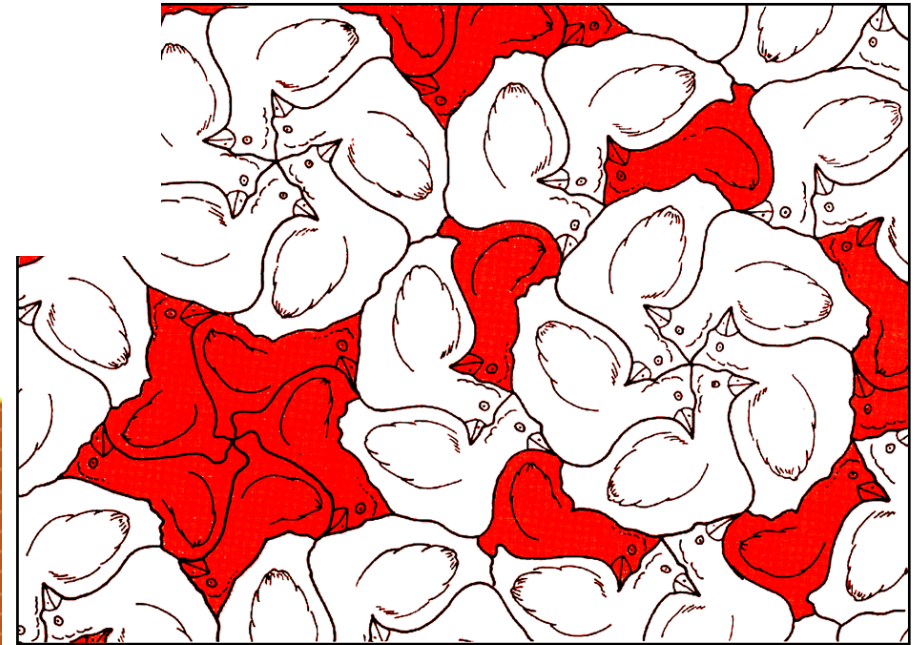
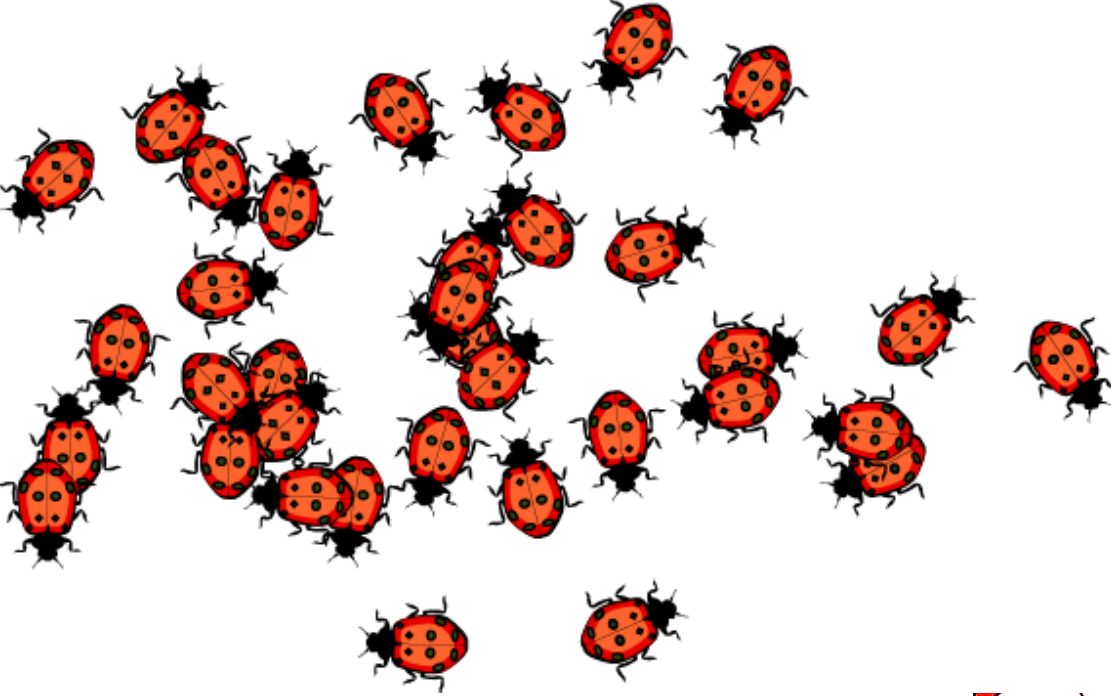


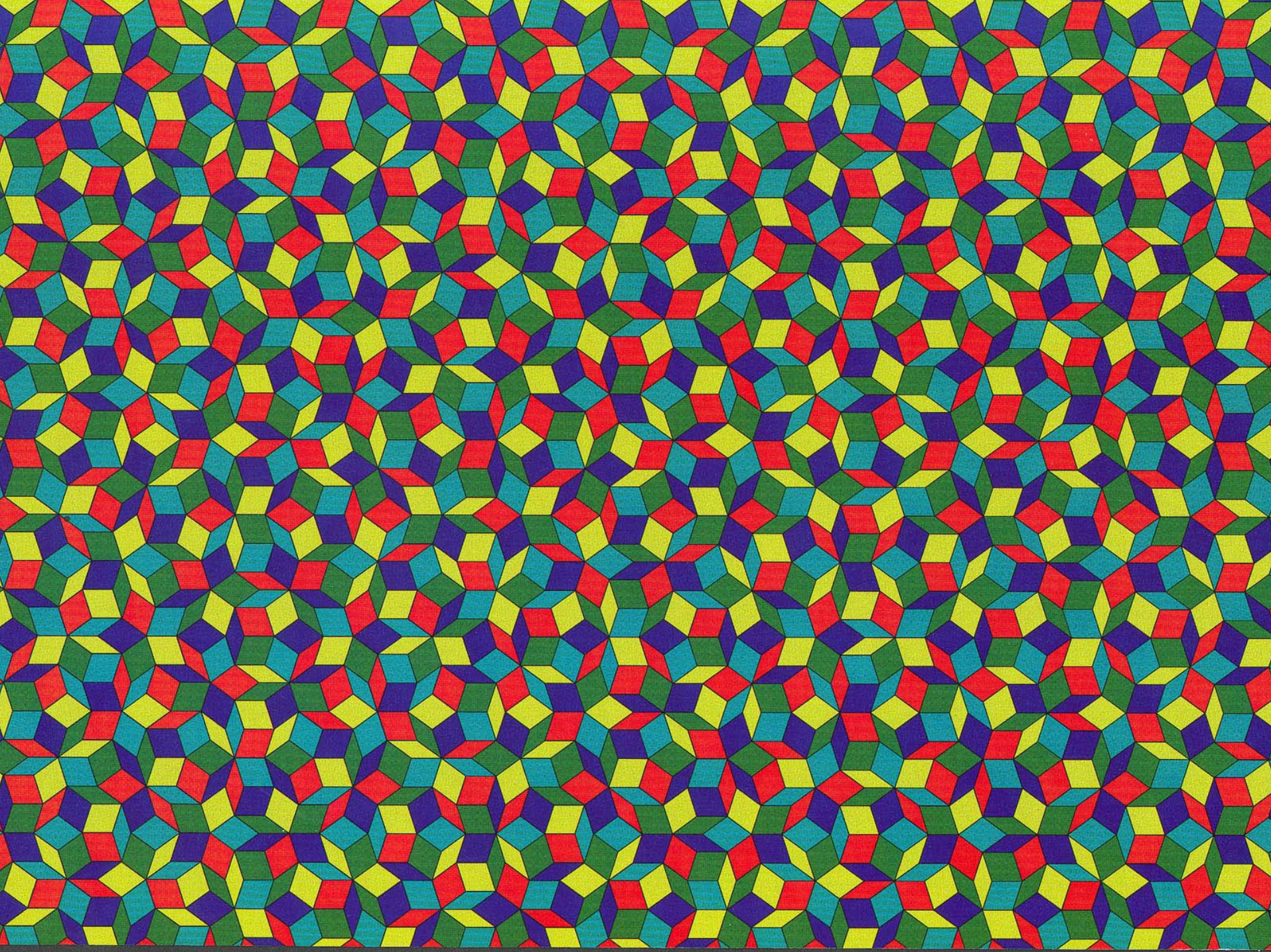
Structure property relationships

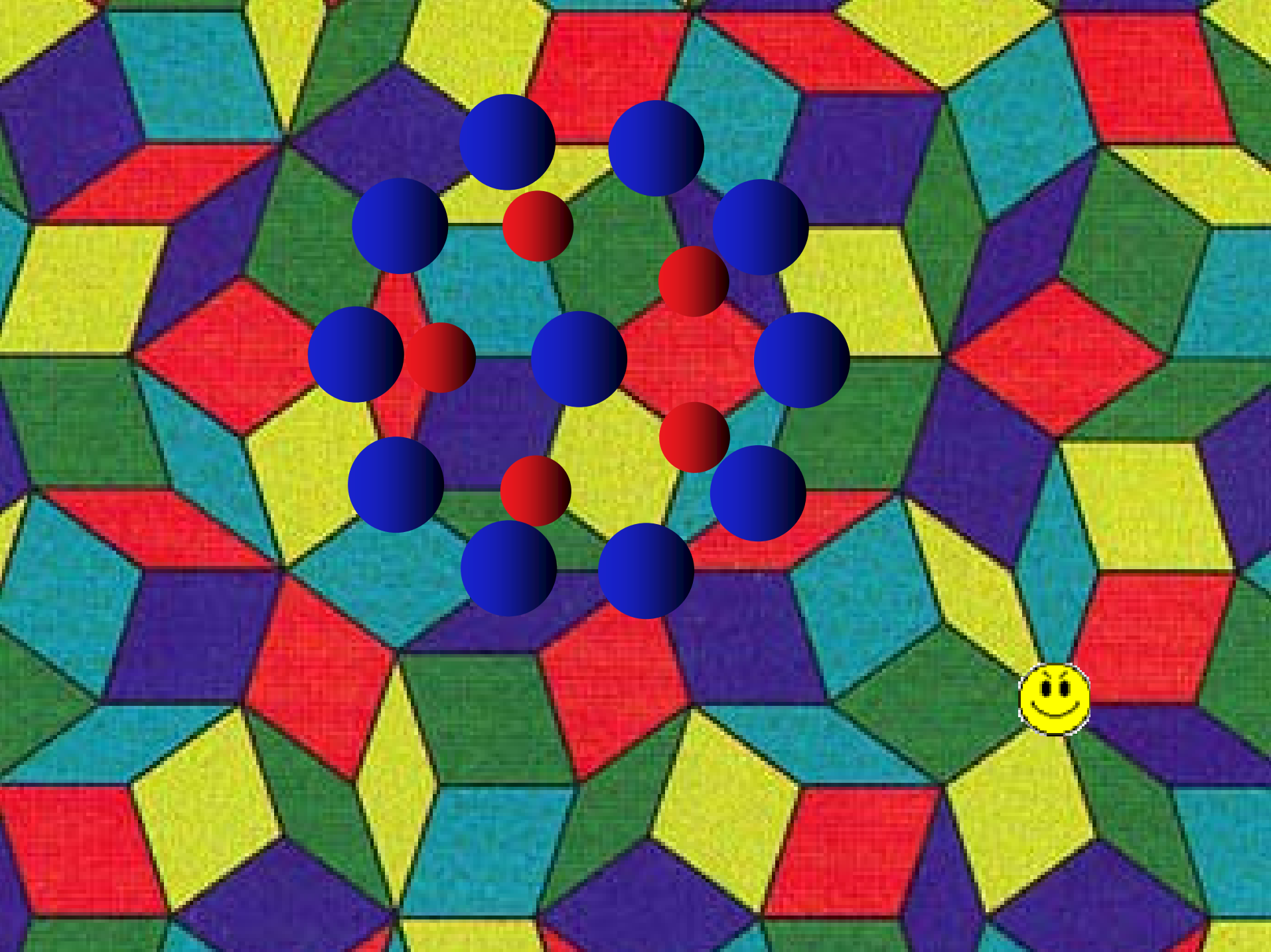


What is a quasicrystal?

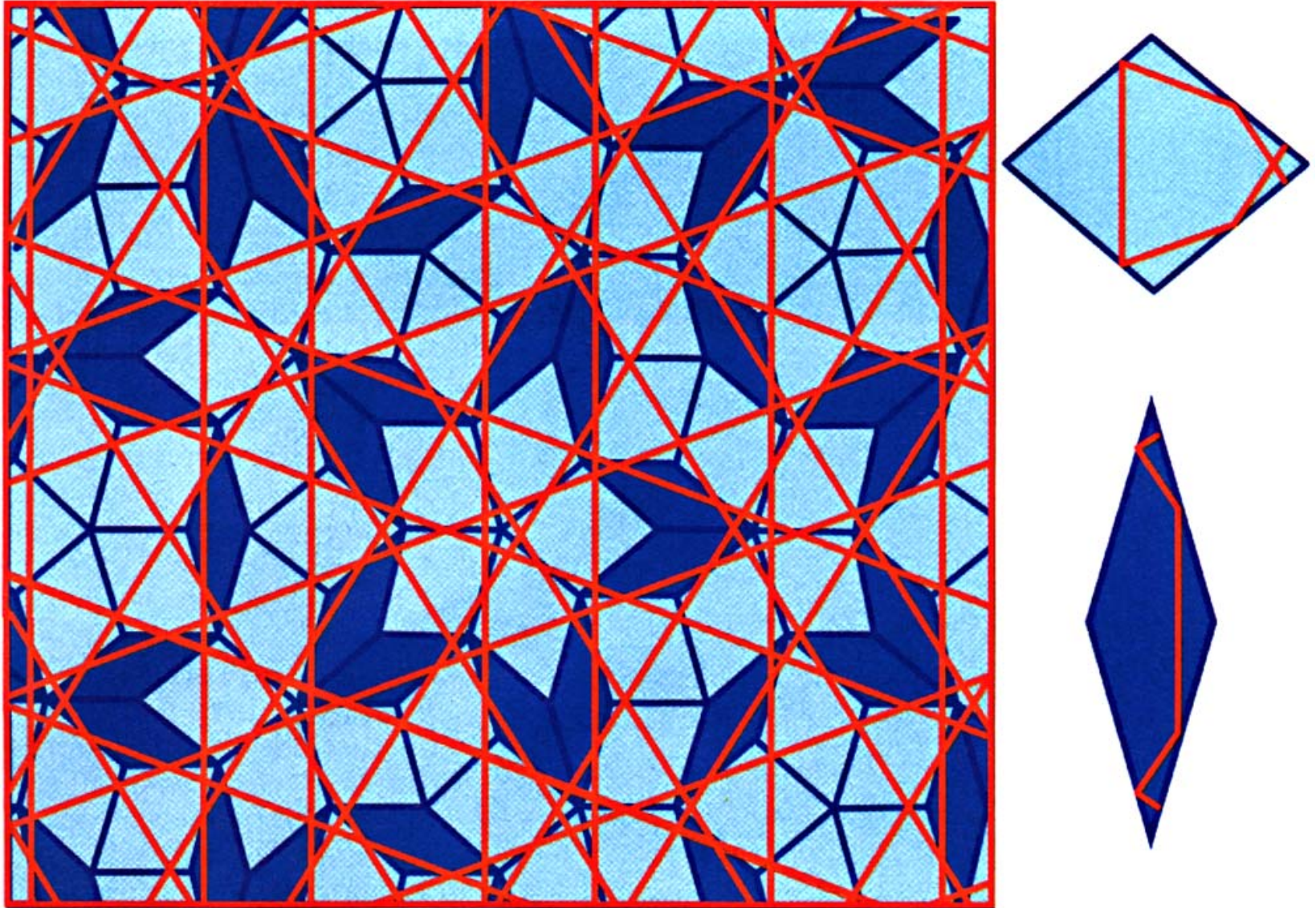
Ordering states





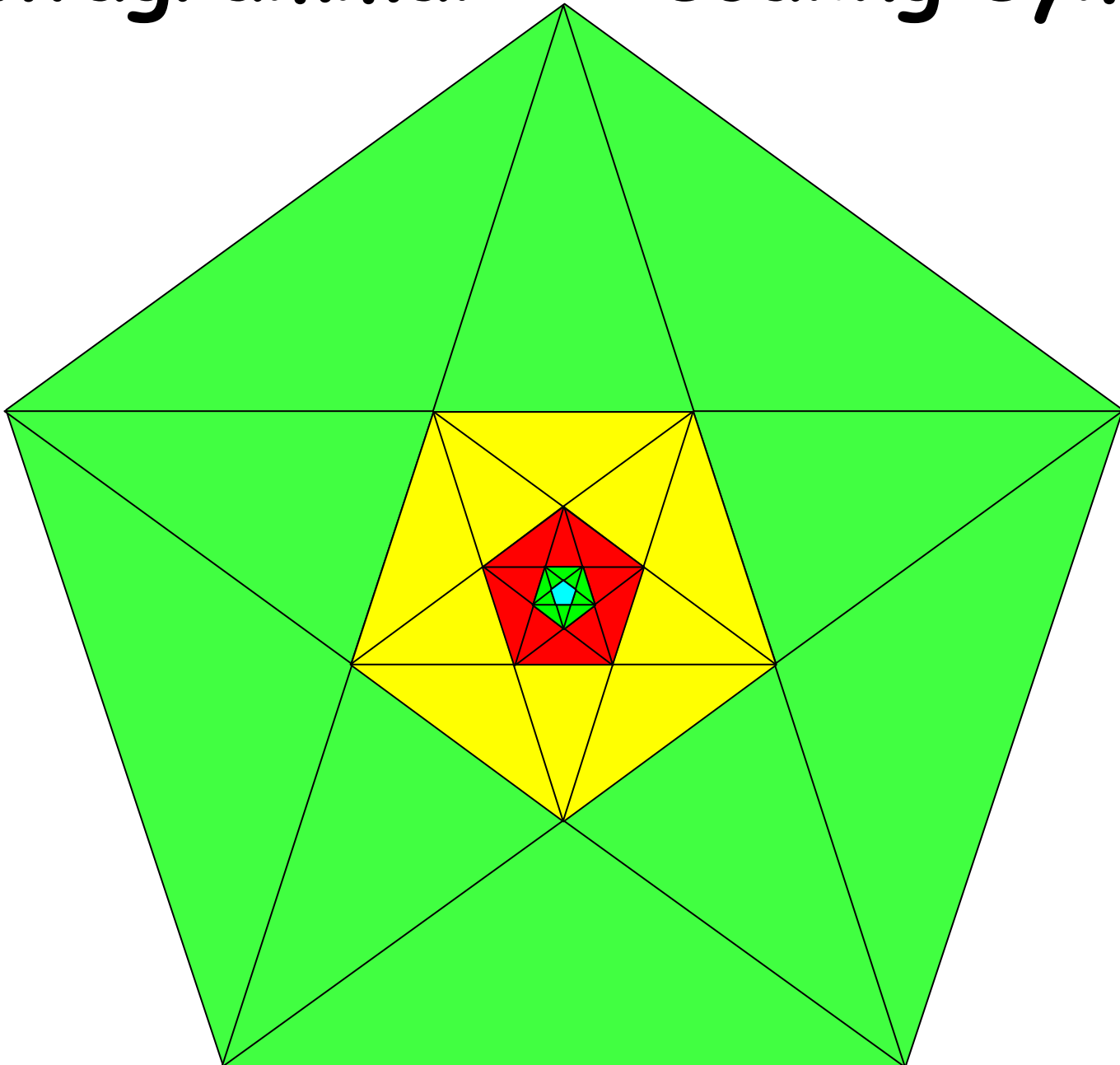


Penrose tiling and Ammann lines



Pentagrammal

scaling symmetry



1

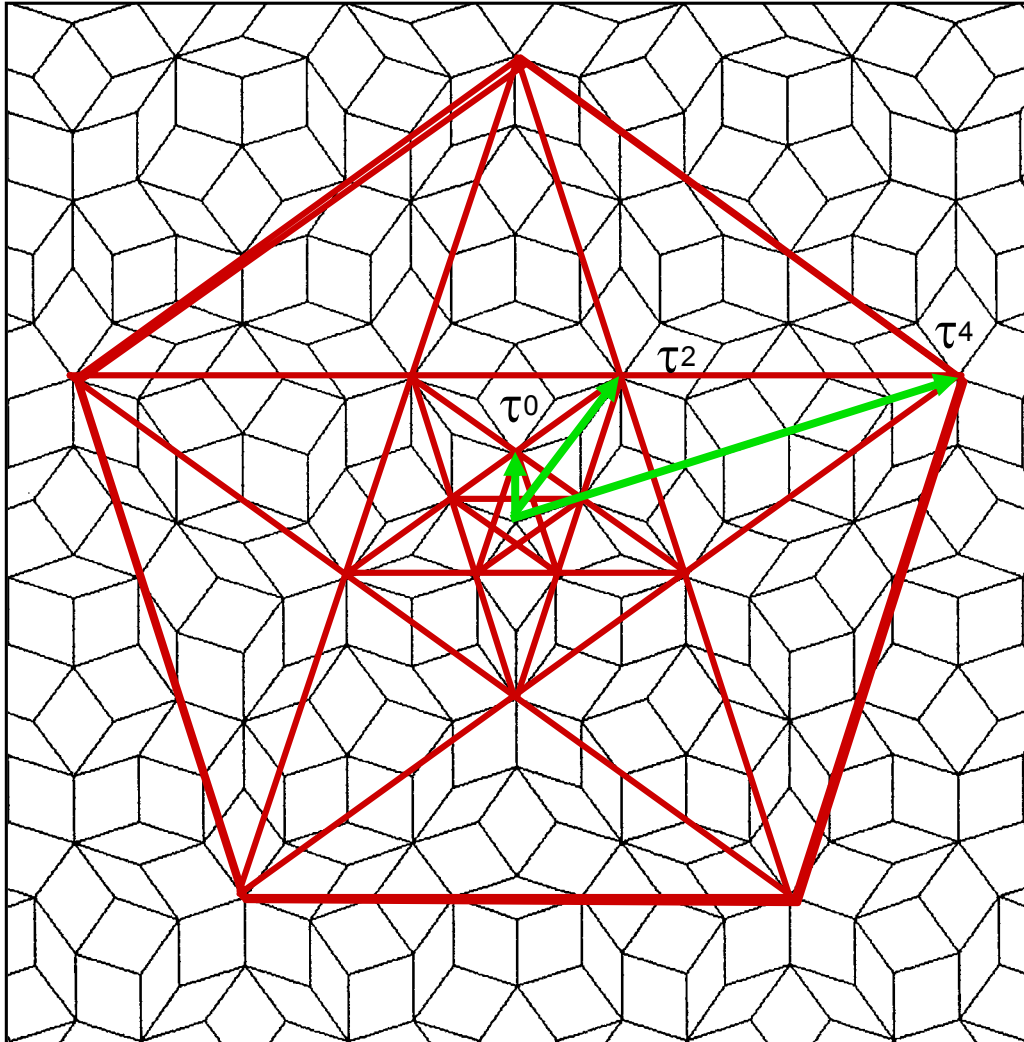
τ^{-2}

τ^{-4}

τ^{-6}

τ^{-8}

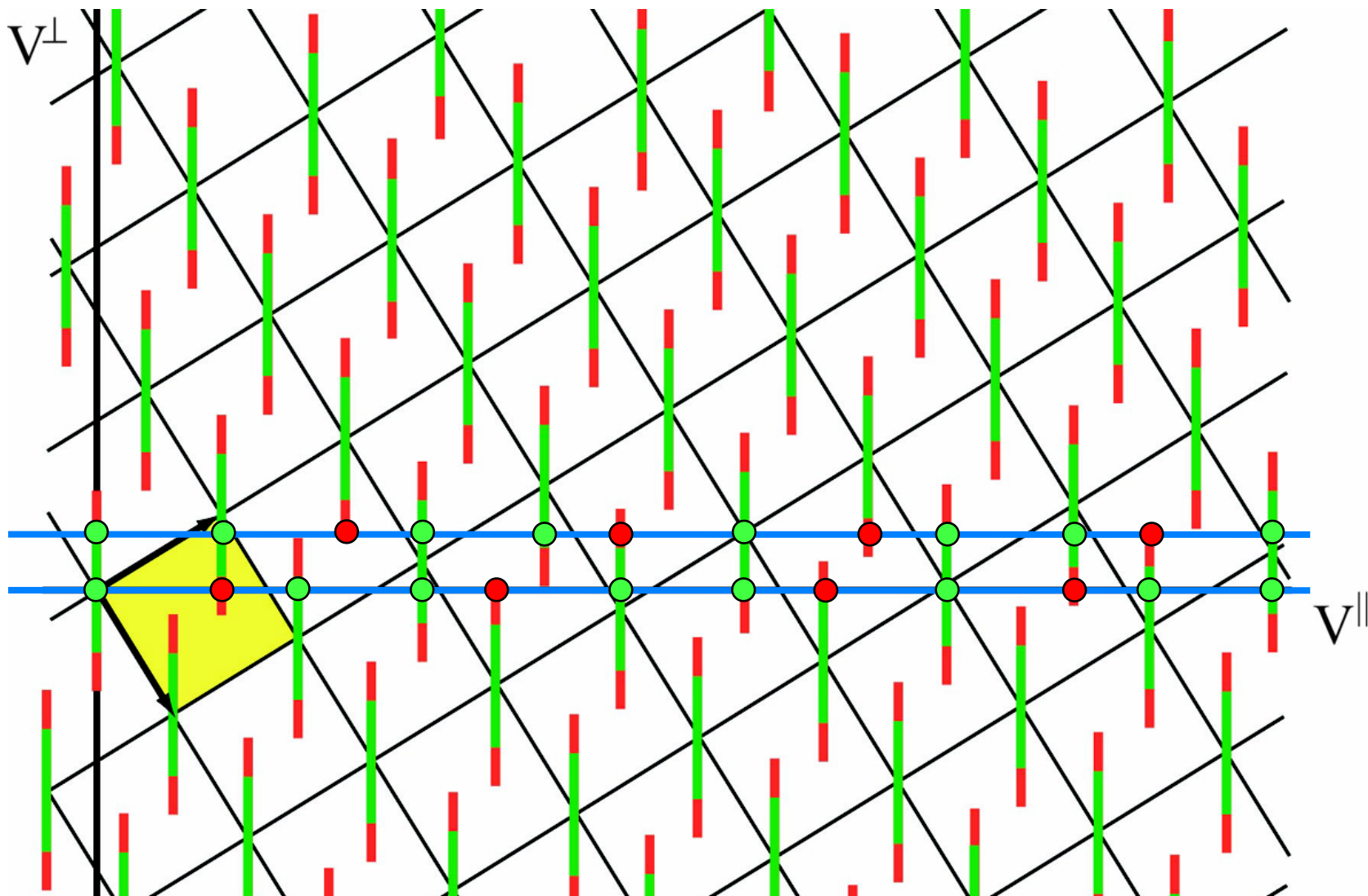
Pentagrammal scaling symmetry



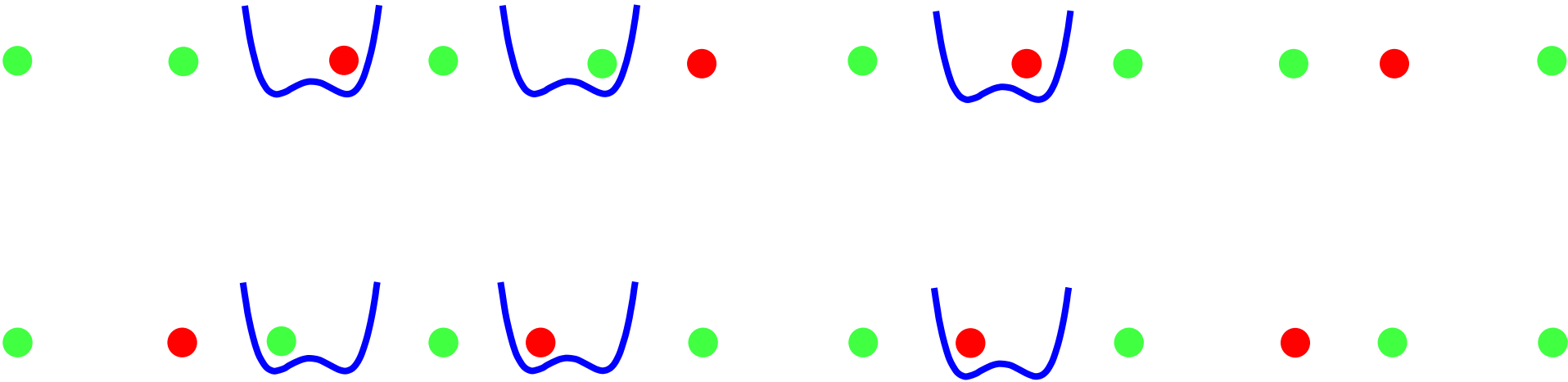
Higher-dimensional modelling of atomic structure and order/disorder phenomena of quasicrystals

Higher-dimensional description

● L ● L ● S ● L ● S ● L ● L ● S ● L ● S ● L ●
● L ● S ● L ● S ● L ● L ● S ● L ● L ● S ● L ●

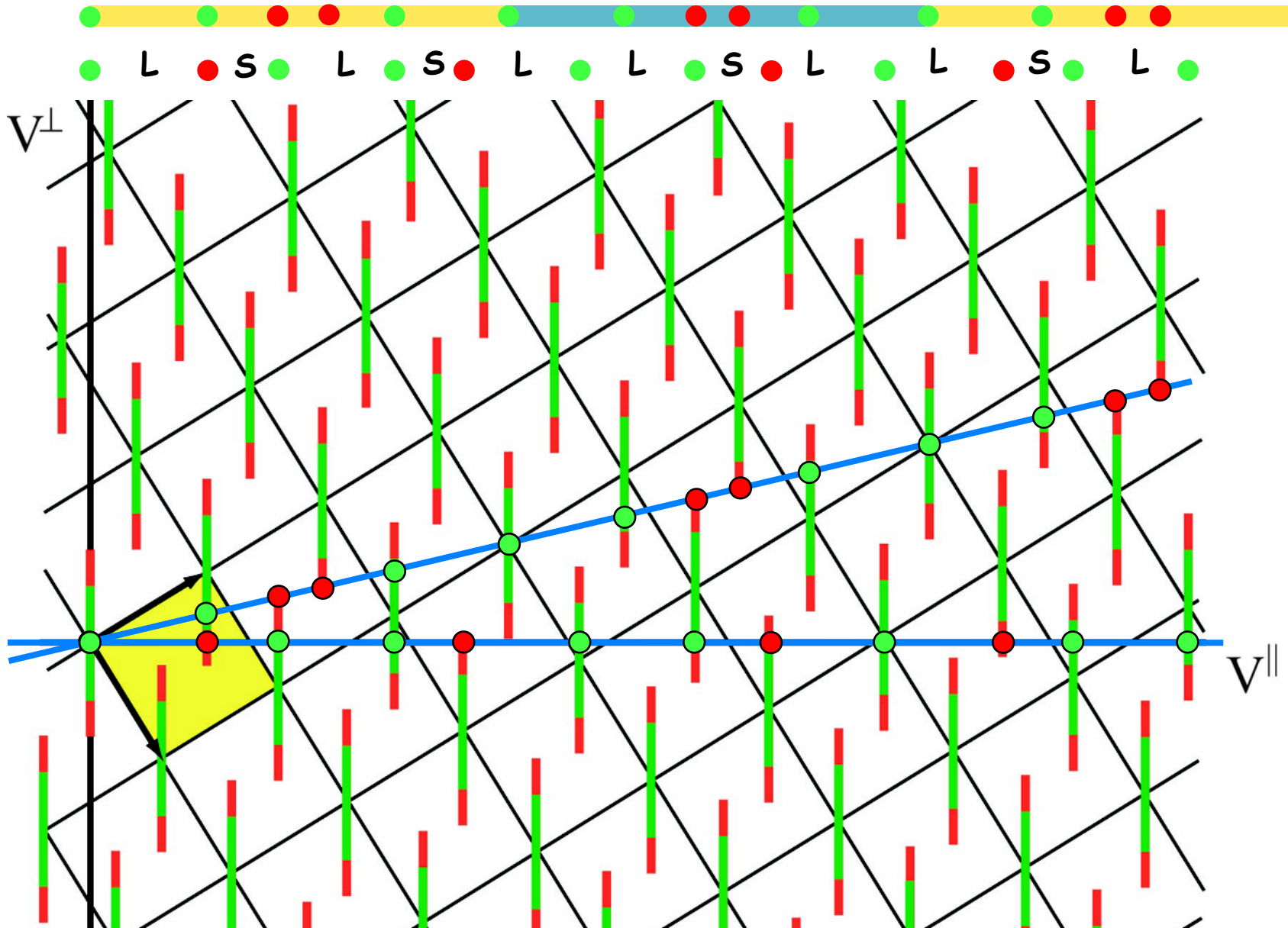


Phason flips of the Fibonacci chain

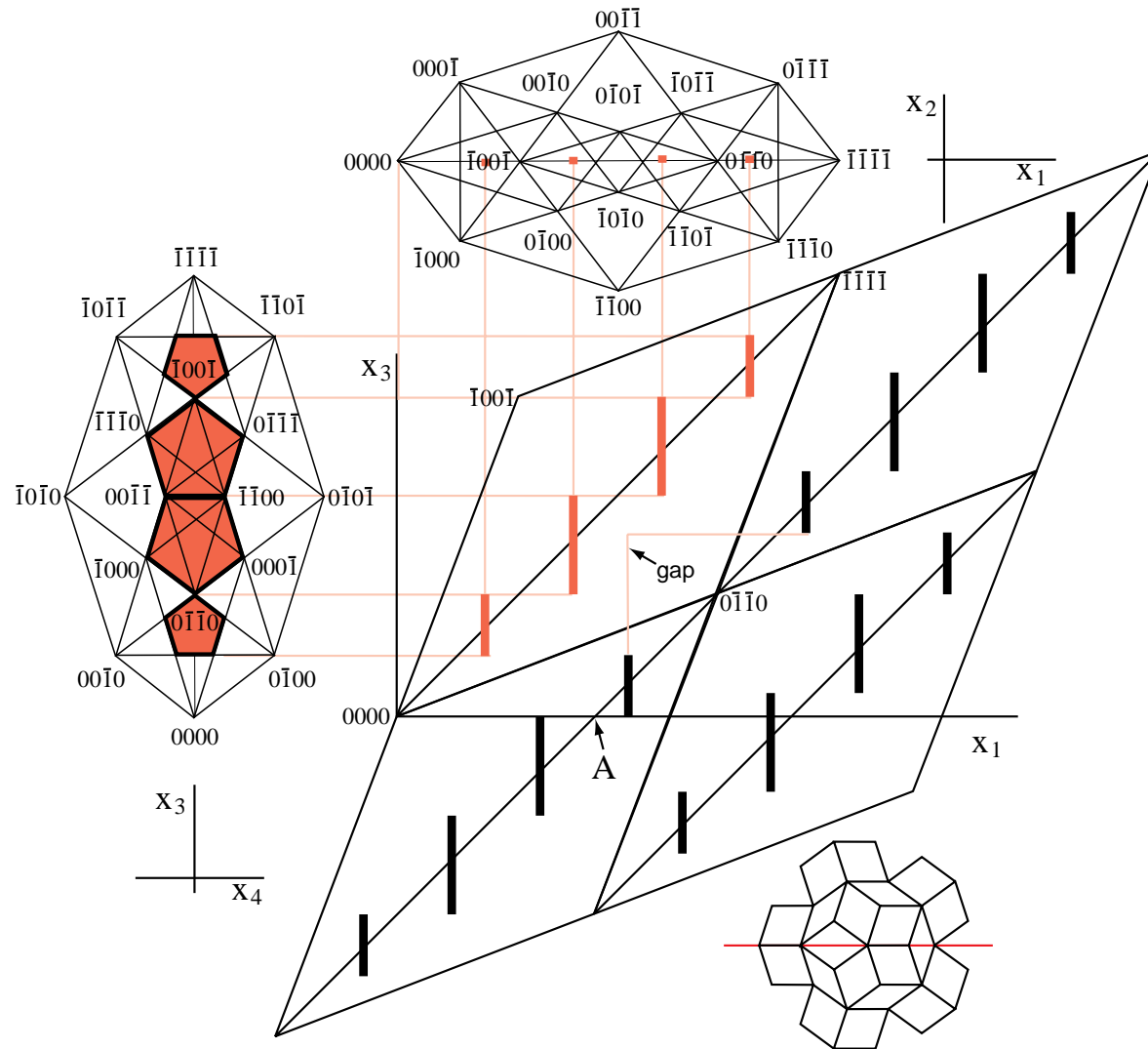


Double-well potential with low energy barrier

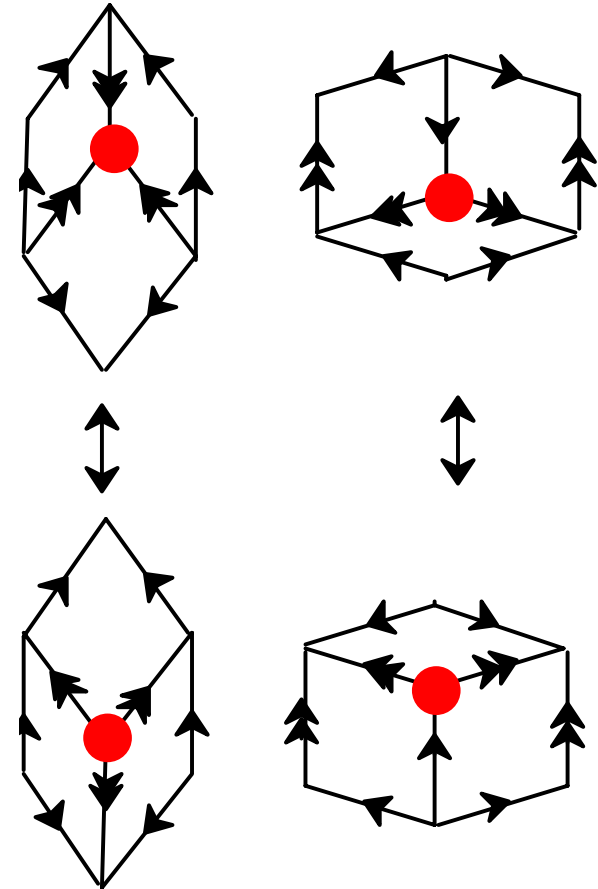
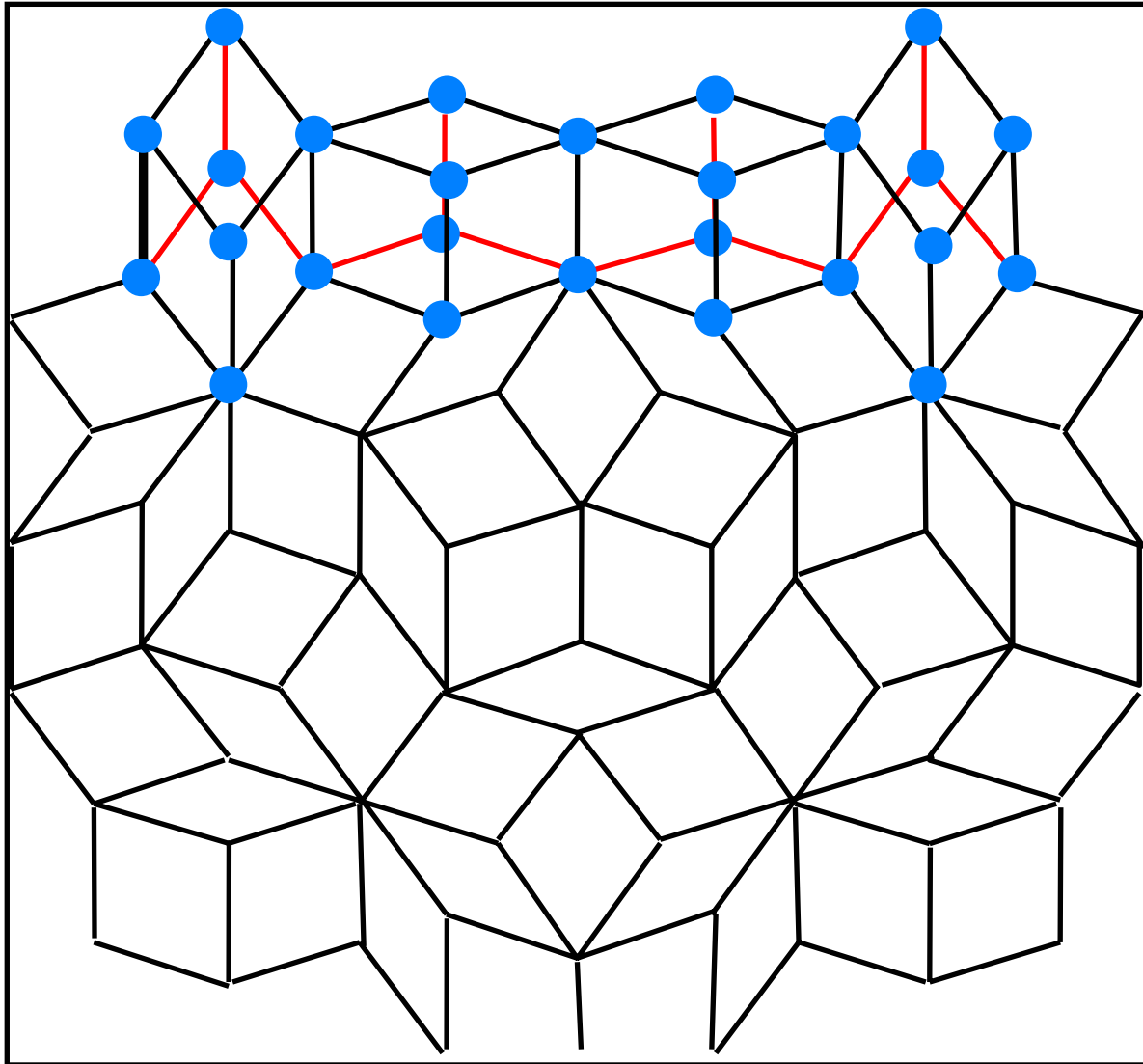
Higher-dimensional description



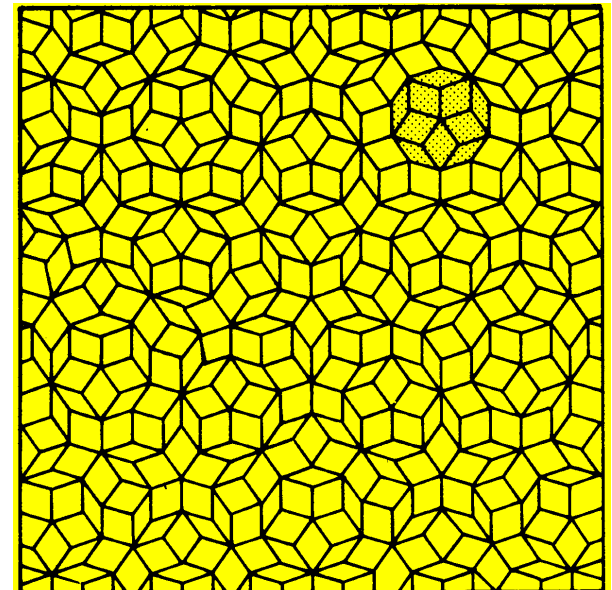
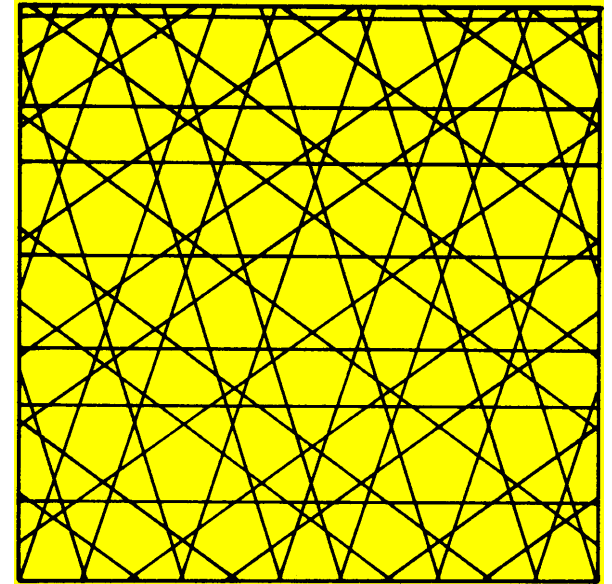
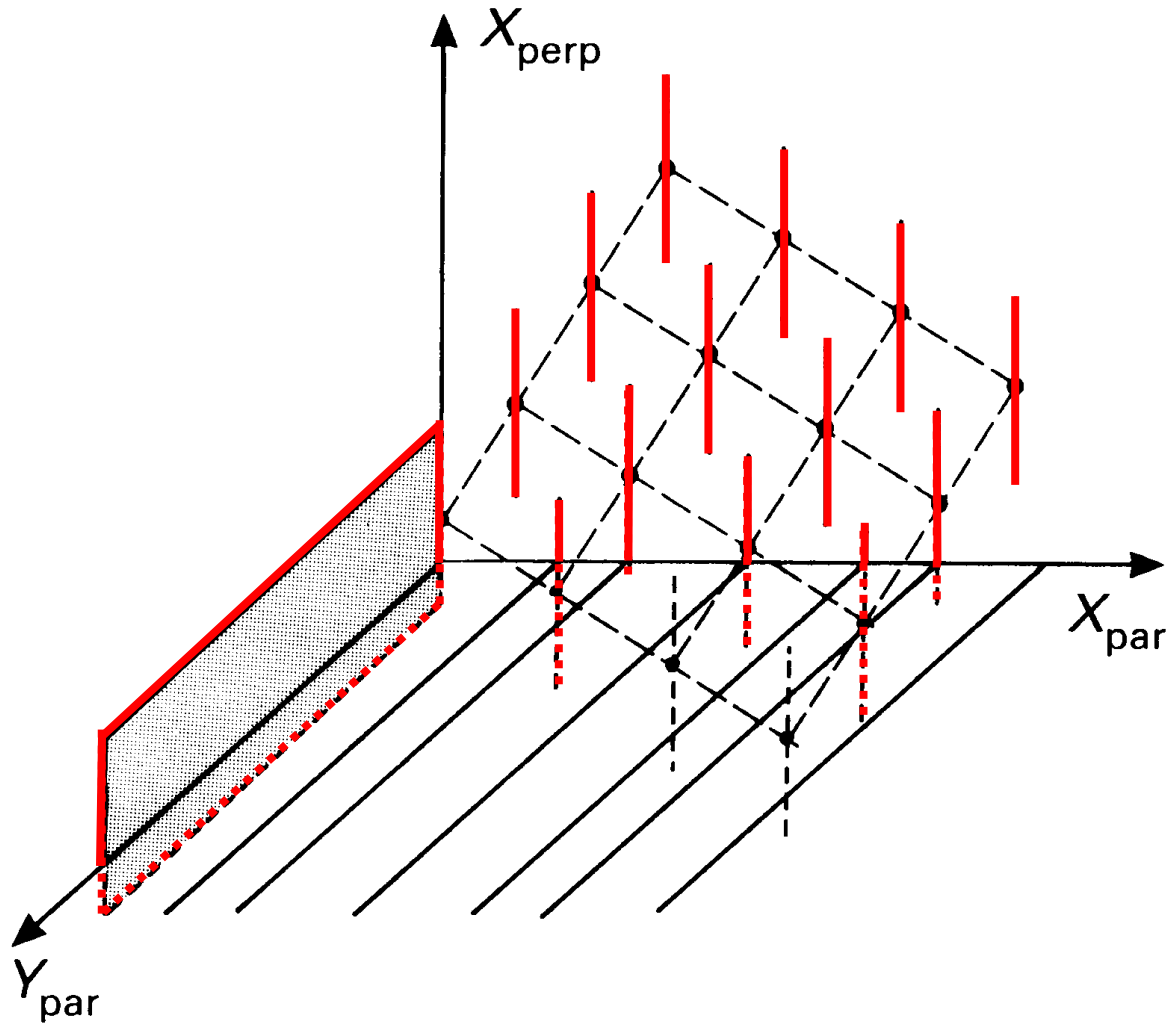
The Penrose tiling in the 4D-description



Phason flips of the Penrose tiling

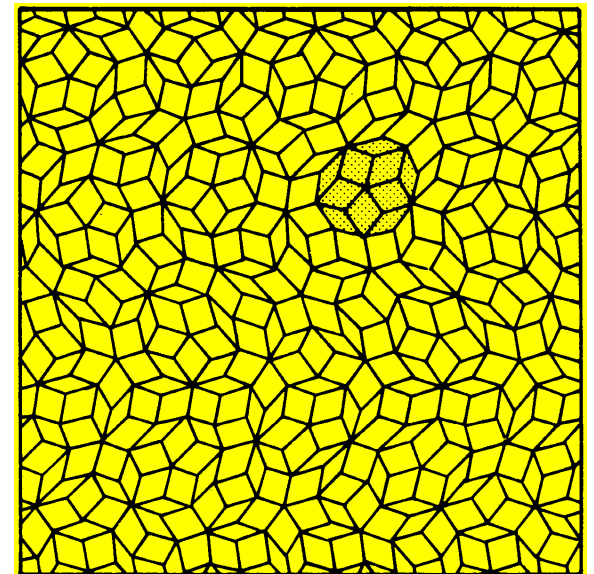
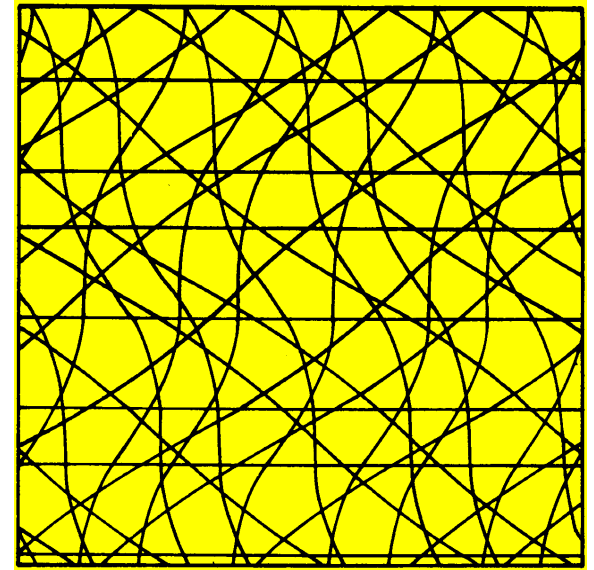
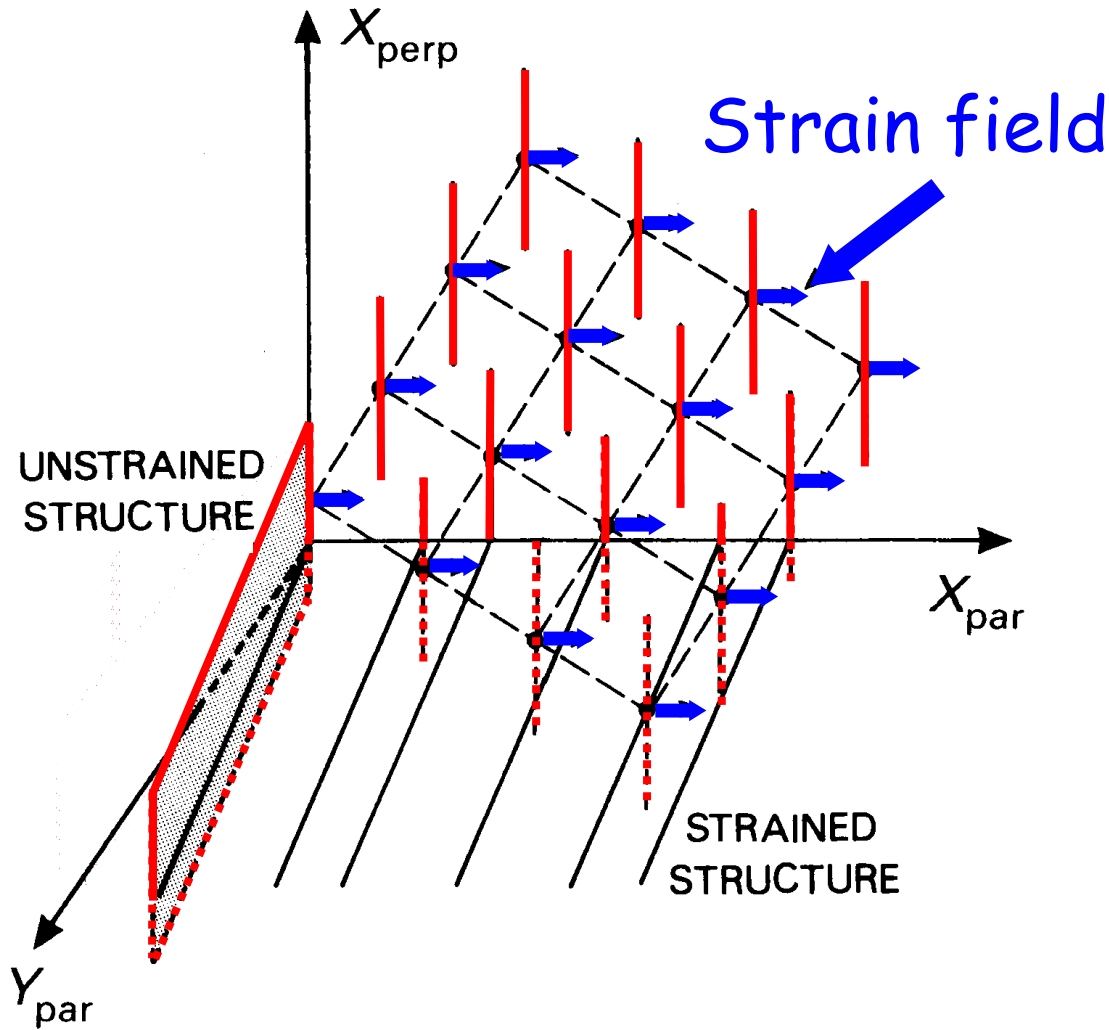


Phonon and Phason Strain



unstrained (Janot, 1995)

Phonon and Phason Strain



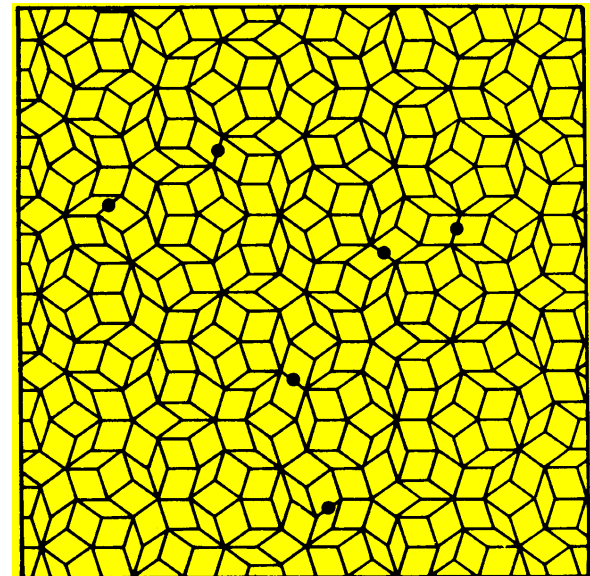
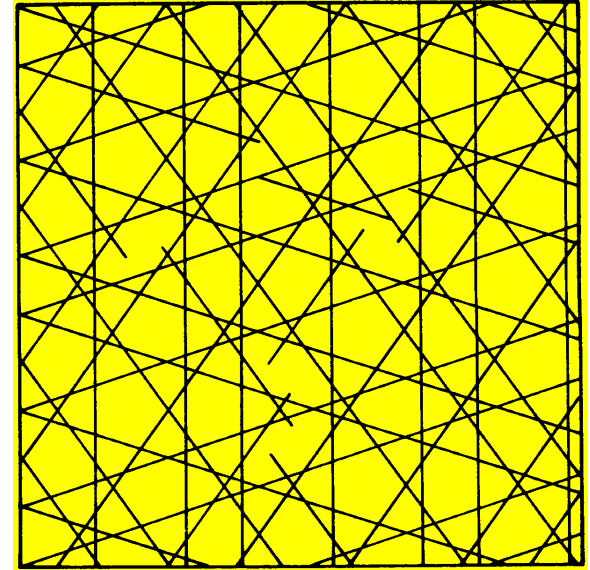
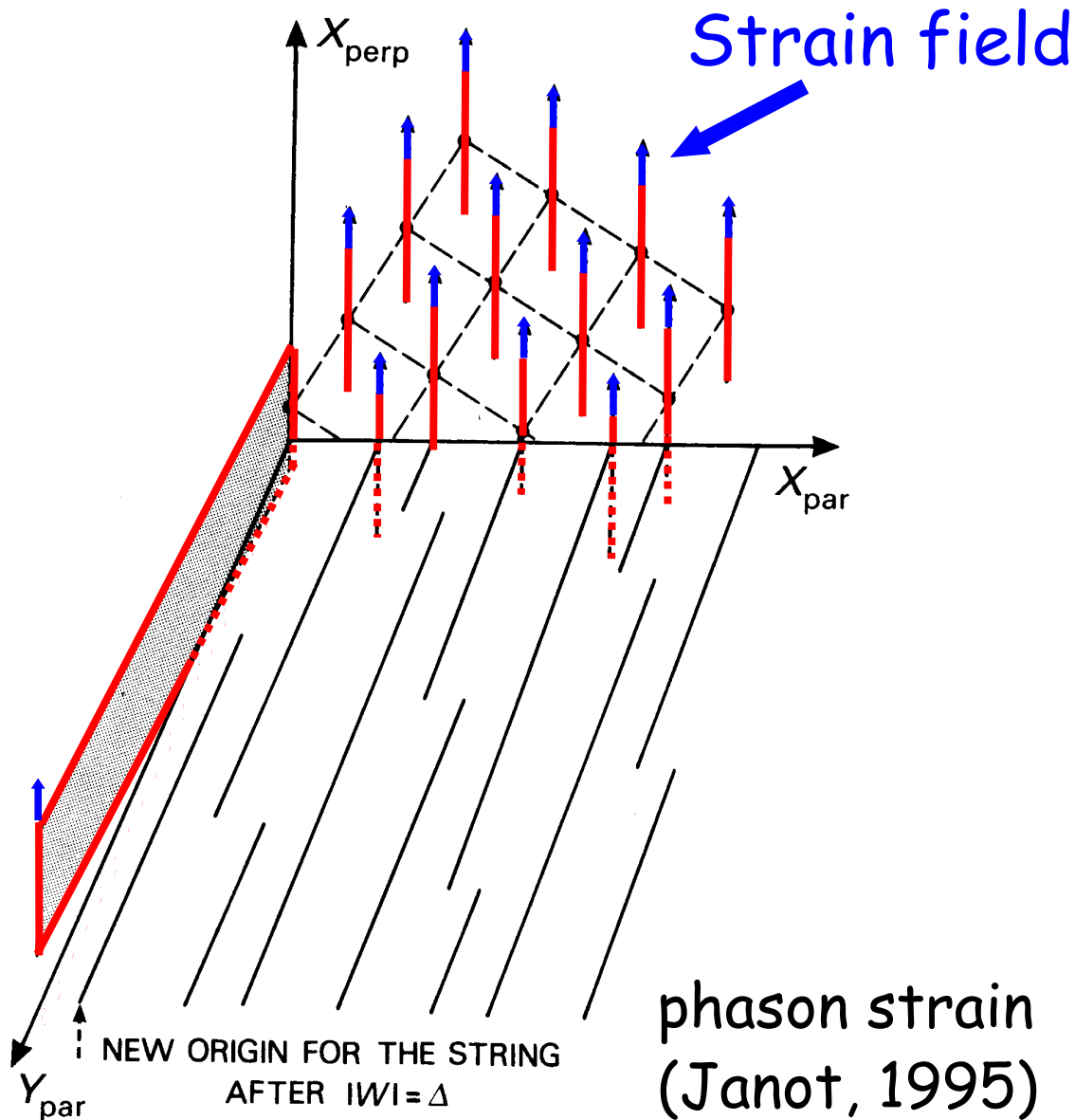
phonon strain (Janot, 1995)

Phonon and Phason Strain

QuickTime™ and a GIF decompressor are needed to see this picture.

phonon strain (Welberry, 2003)

Phonon and Phason Strain



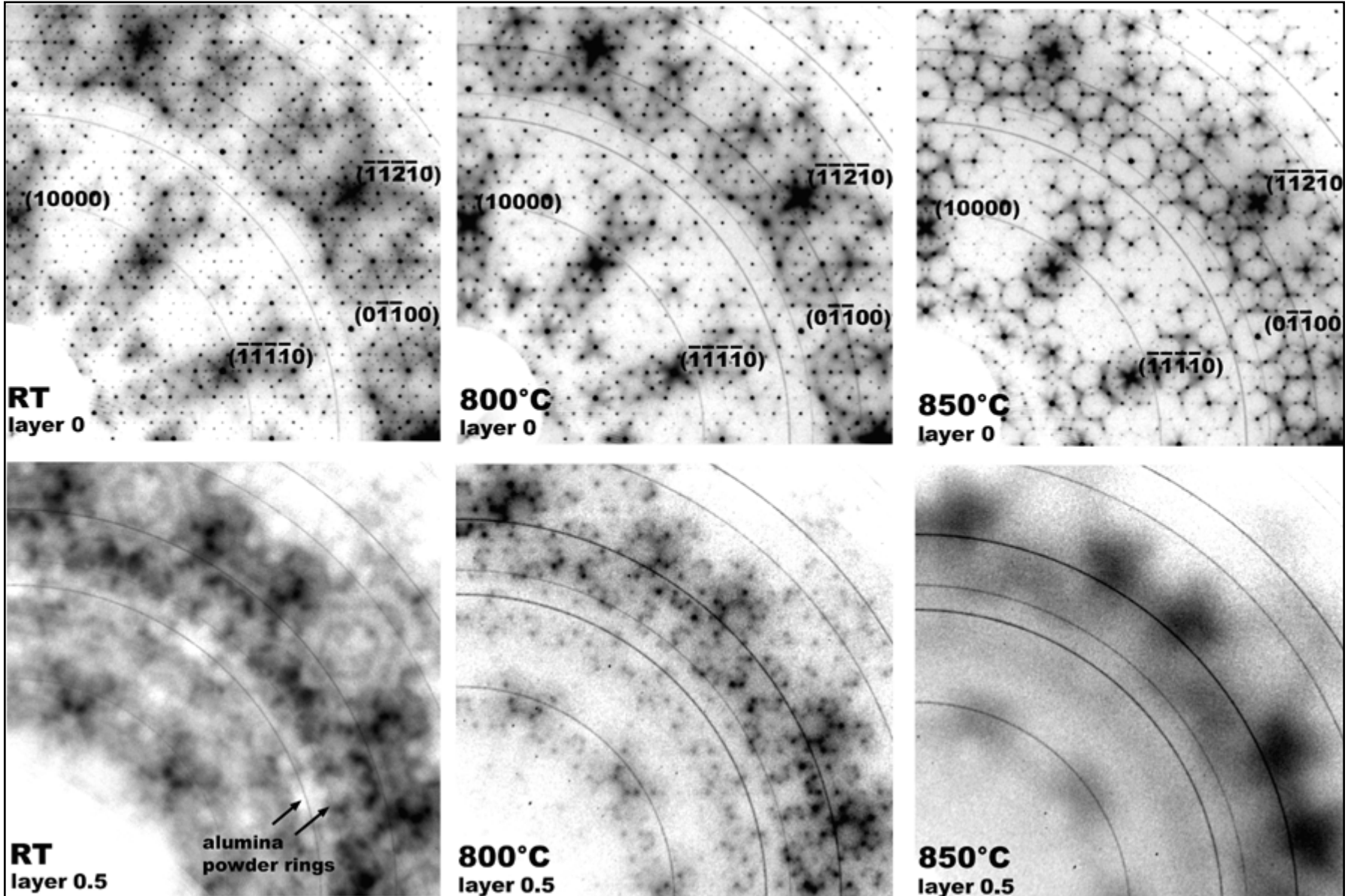
QuickTime™ and a MPEG-4 Video decompressor are needed to see this picture.

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HT-Diffraction data of d-Al-Co-Ni



Structure analysis of Quasicrystals

Regular crystal structure analysis:
determination of short-range order
(atomic arrangement in one unit cell).

Quasicrystal structure analysis:
determination of both short- and long-
range order (structure of "clusters" as
well as "cluster" ordering).

Fundamental questions



What governs formation and stability of quasicrystals?



Are quasicrystals energy or entropy stabilized phases (a ground state of matter)?



Are quasicrystals quasiperiodic?

What governs formation and stability of approximants and quasicrystals?

- Chemical composition?
- Valence electron concentration?
- Vacancy concentration?
- Positional and/or substitutional disorder?
- Temperature and/or pressure?

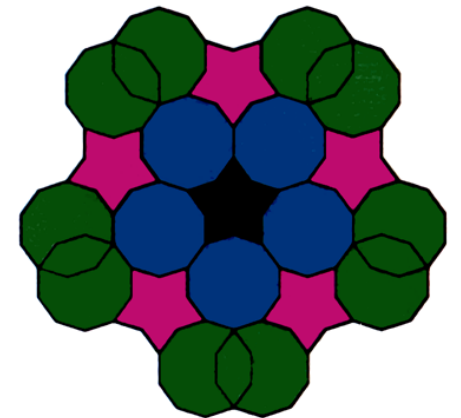
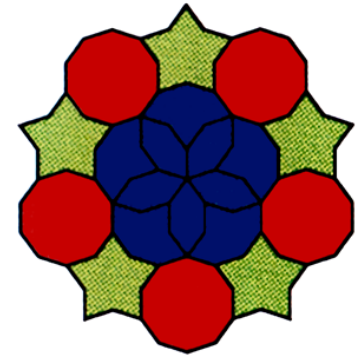
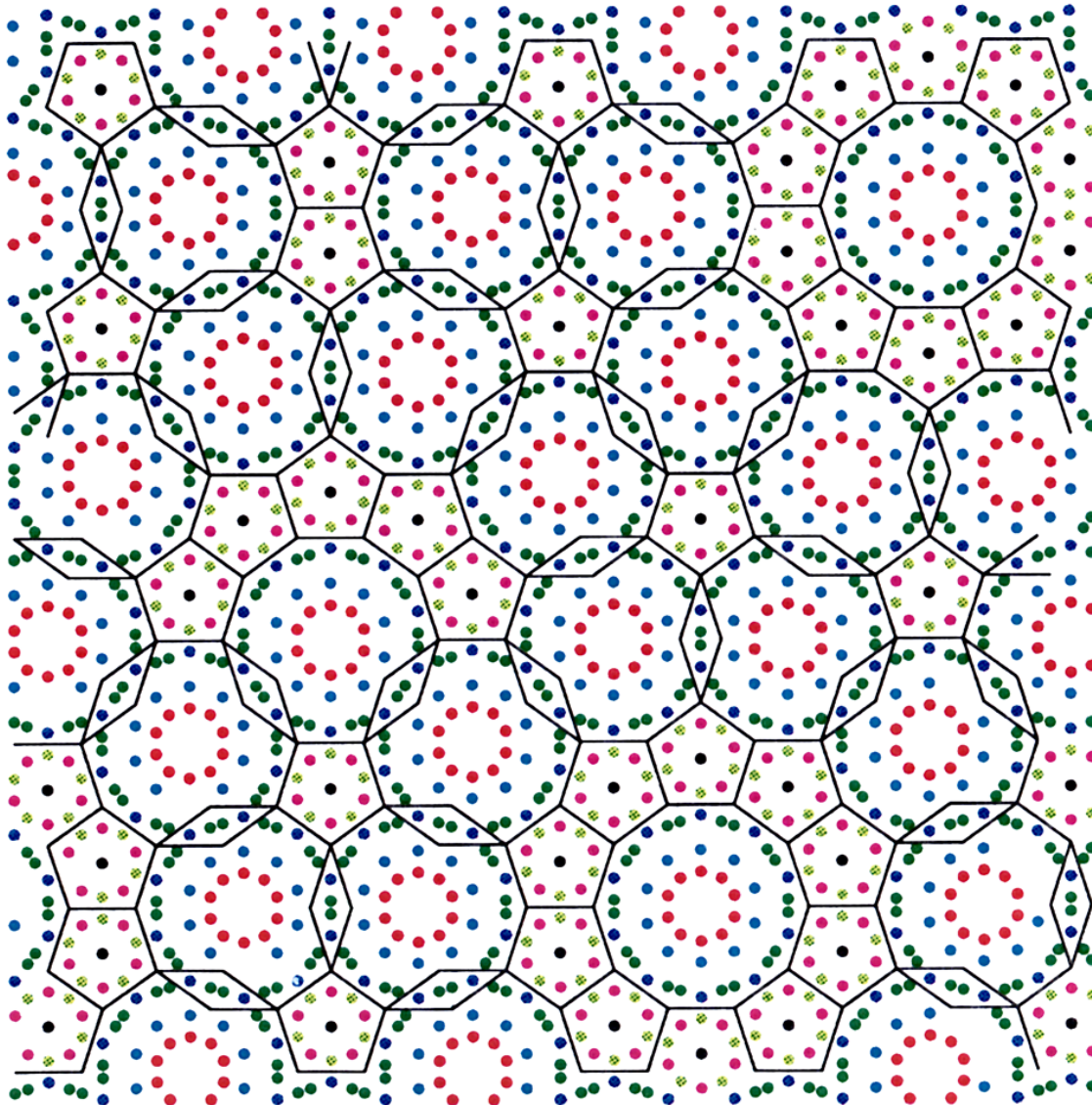
Are quasicrystals energy or entropy stabilized phases (a ground state of matter)?

- Variation of structure as a function of temperature, pressure?
- Thermodynamic parameters as a function of temperature, pressure?
- Quantum-mechanical calculations

Are quasicrystals quasiperiodic?

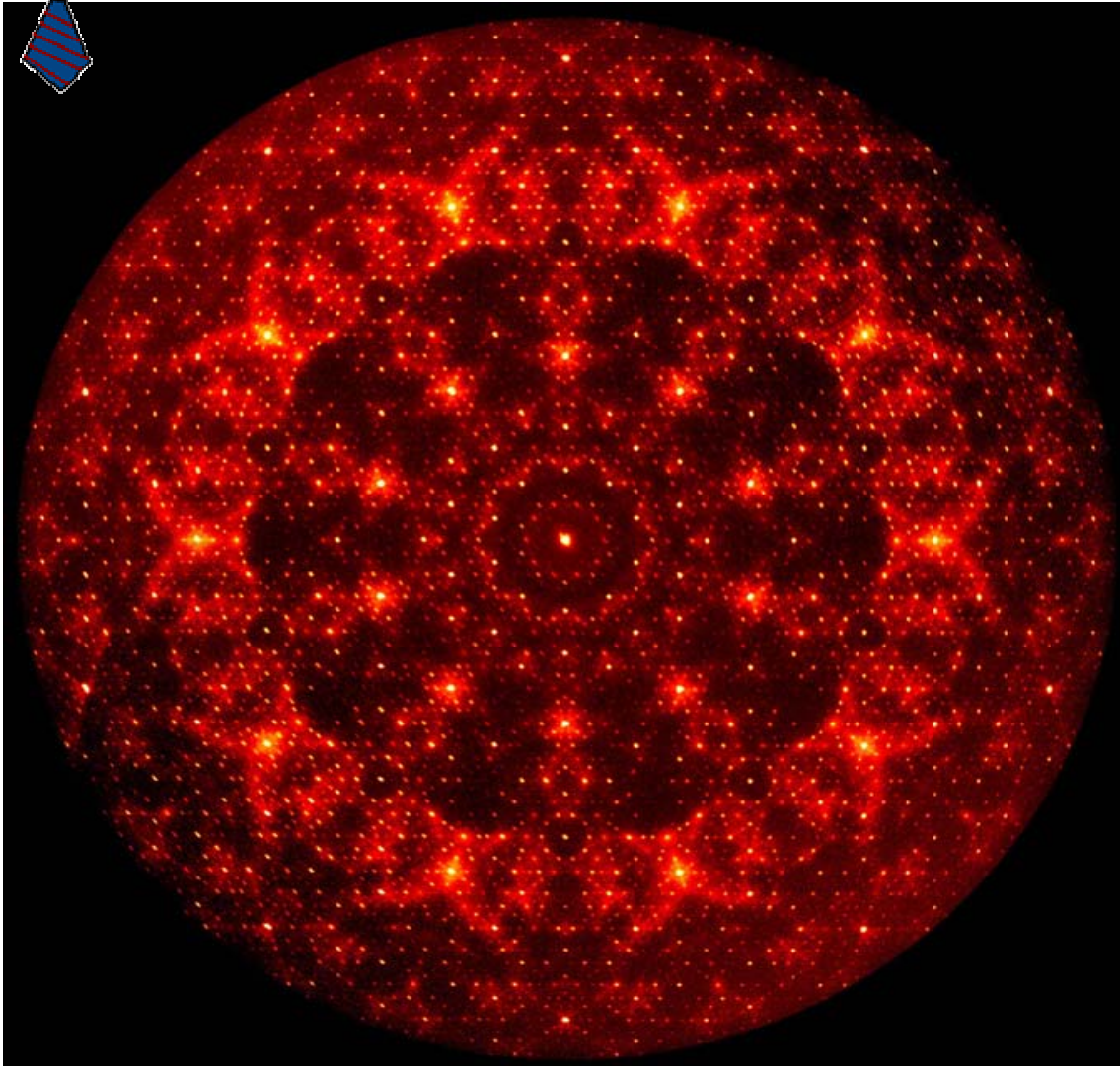
- Strictly quasiperiodic?
- On average quasiperiodic?
- nD description appropriate?
- Dependence on temperature, pressure?

Model of decagonal Al-Co-Ni



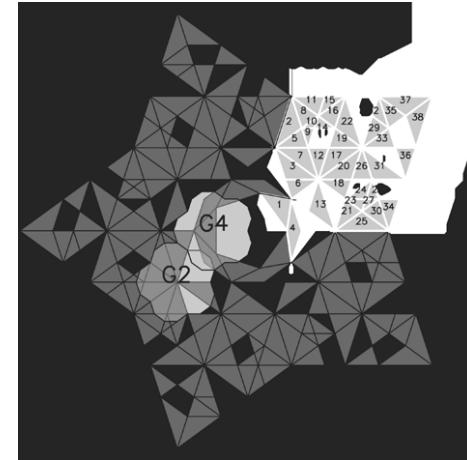
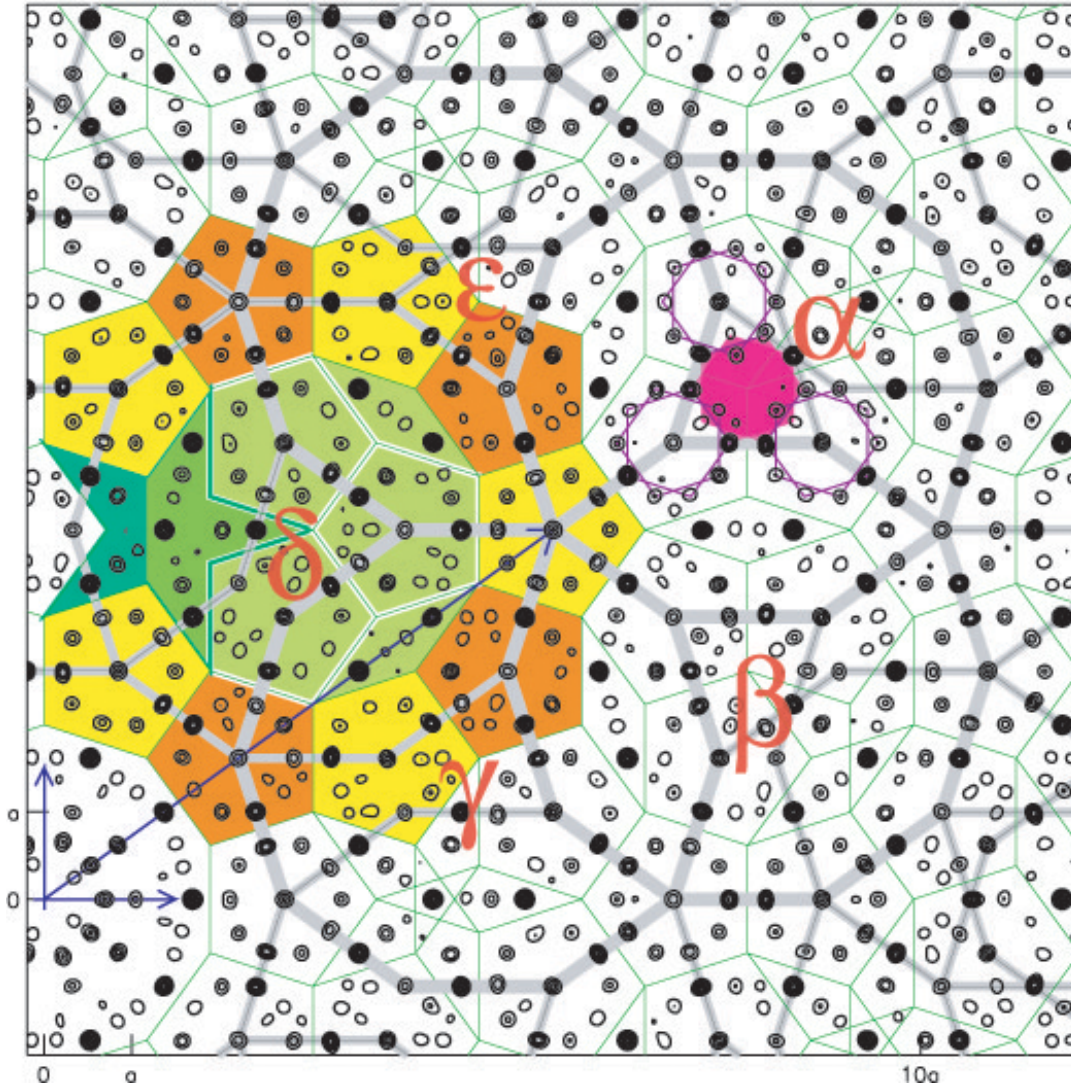
Yamamoto (1996)

Reciprocal space reconstruction



Second tenfold reciprocal lattice layer of decagonal Al-Co-Ni reconstructed from 720 single frames (0.25° oscillation range each, SNBL/ESRF).

Decagonal $\text{Al}_{70.6}\text{Co}_{6.7}\text{Ni}_{22.7}$



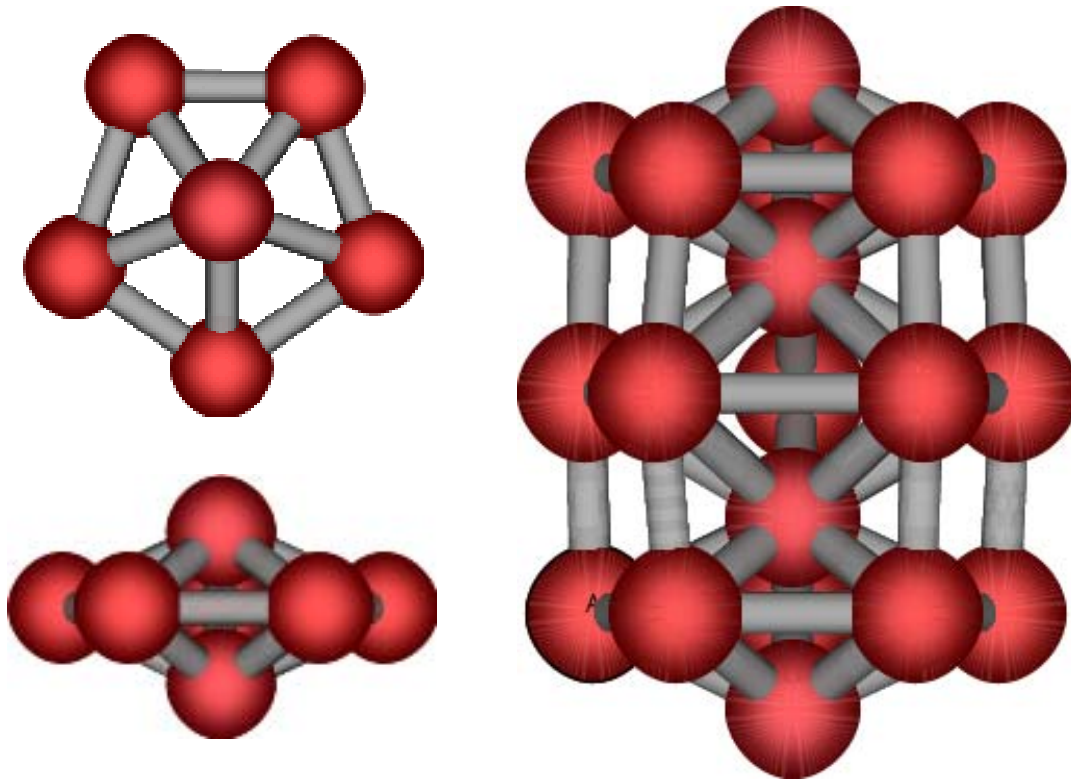
40Å x 40Å projection of a high-resolution electron density map with overlying pentagonal Penrose tiling (Niizeki modification).



QuickTime™ and a Video decompressor are needed to see this picture.

$Pnm2_1$ (No 31), $a=8.158(1)$ Å, $b=12.342(1)$ Å, $c=14.452(2)$ Å (Grin et al., 1994)

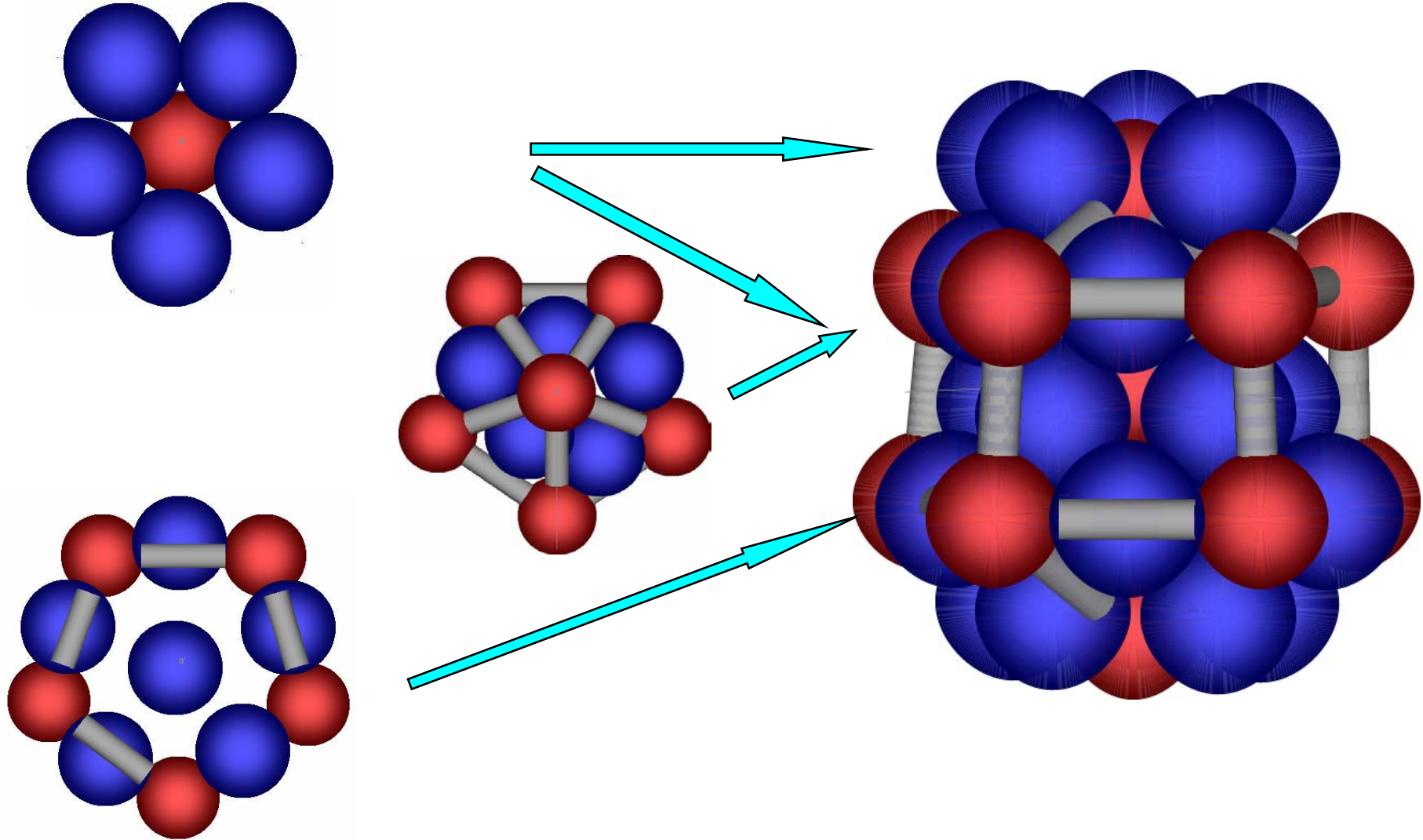
Pentaprisms and Pentagonal Bipyramids



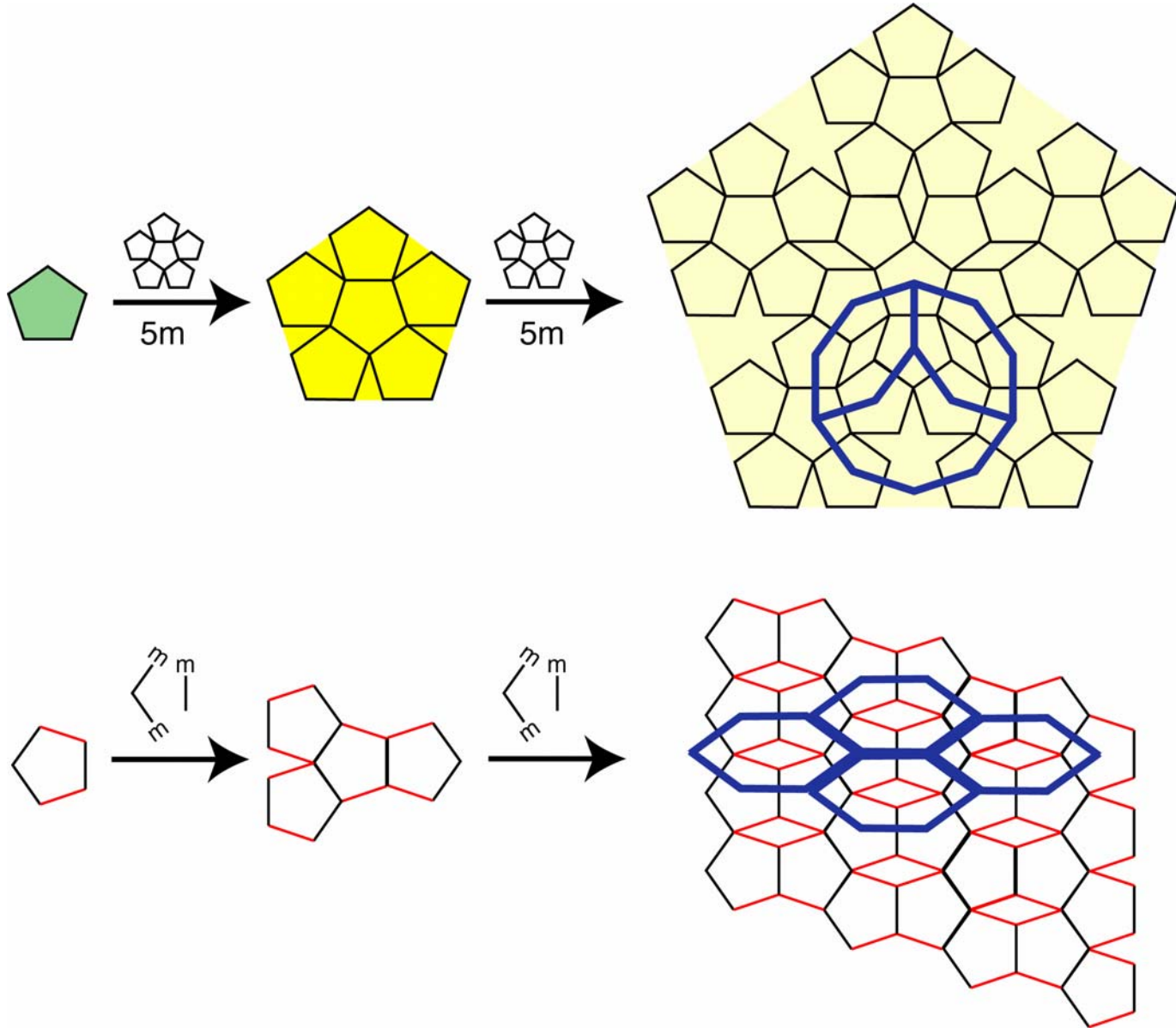
Typical cluster of $o\text{-Al}_{13}\text{Co}_4$.

A PBP of equal spheres is denser locally than any close sphere packing. Note that the spheres in the equatorial layer do not touch. (Cockayne & Mihalkovic, 1999)

Pentaprisms and Pentagonal Bipyramids



Growth of pentagon tilings



Structural Modelling - Where are the atoms and why?

A subset of atoms of Al-based quasicrystals is perfectly quasiperiodically ordered, another subset shows a high degree of mainly phasonic disorder (entropic contribution).

The driving force of quasiperiodic order is local fivefold coordination together with global electronic Hume-Rothery-type stabilization as well as the entropic contribution.