非周期的な構造のフーリエ展開：準結晶と概周期性

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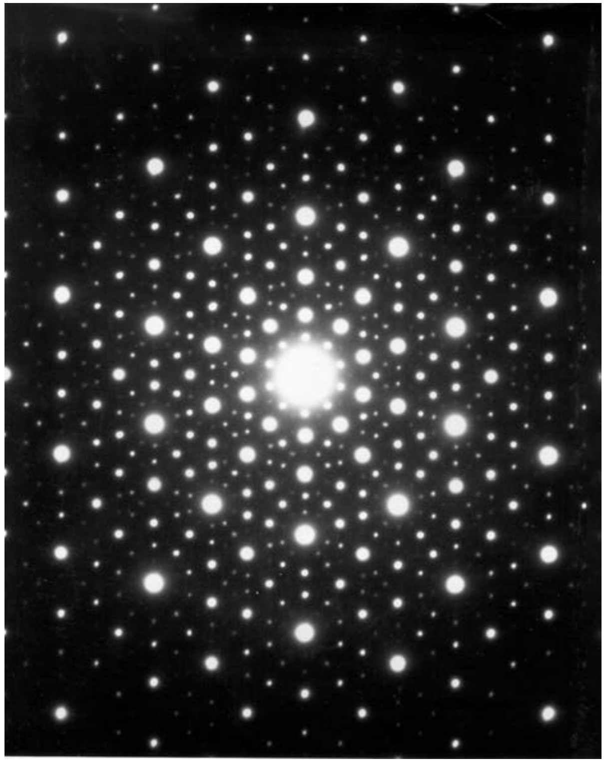
In 1982 Shechtman et al. [5] found Bragg peaks with 10-th fold symmetry in rapidly cooled Mn-Al alloy, which is later called 'quasi-crystal'. Shechtman won 2011 Novel prize by this discovery. Recently a lot of quasi-crystals are found in much larger scale. **Mathematics of Aperiodic Order** is a new branch of mathematics, which aims at giving mathematical models of them.



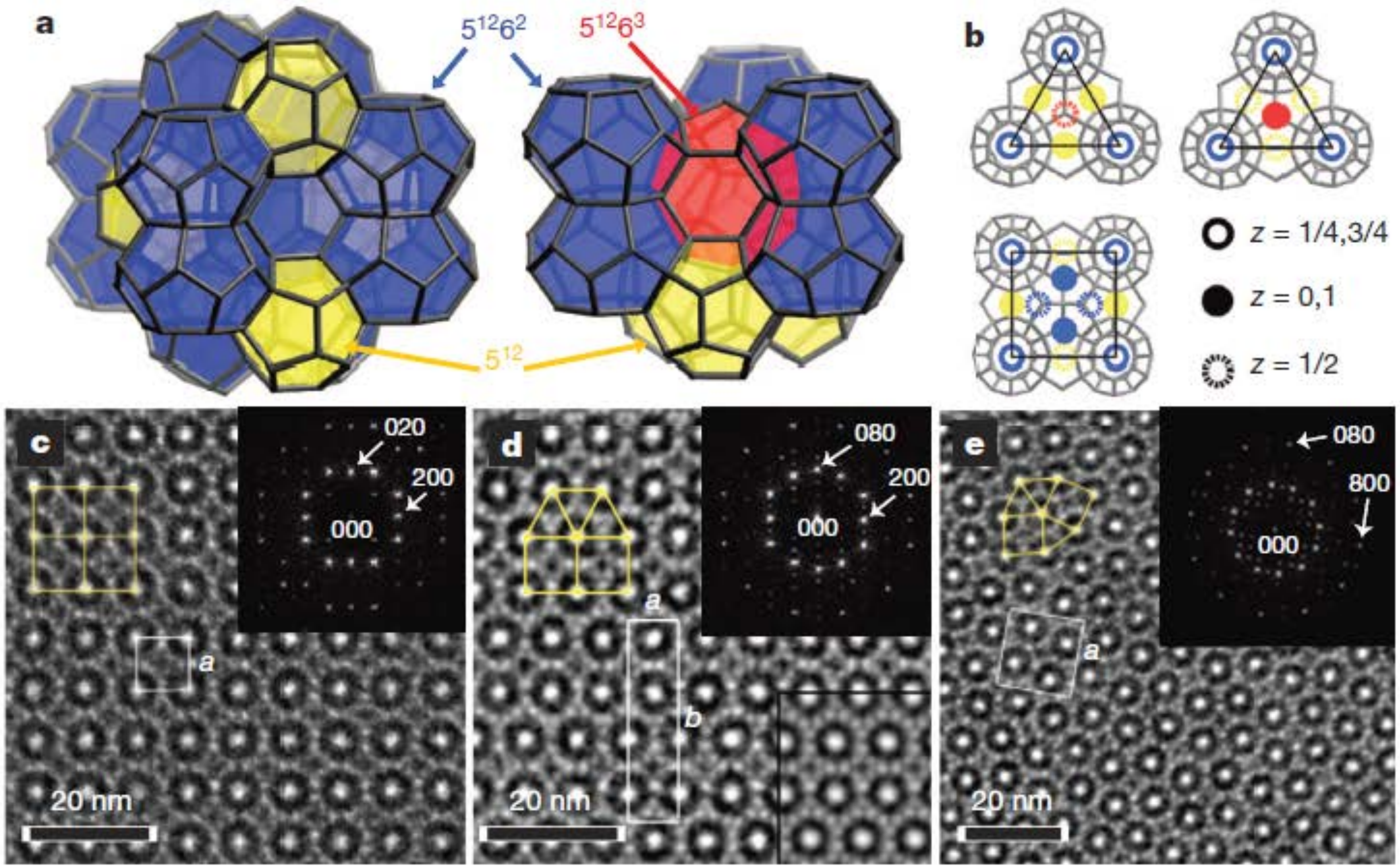


Figure 1: Dodecagonal tiling in mesoporous silica

Nature, Vol 487: 2012, Xiao, Fujita, Miyasaka, Sakamoto, Terasaki

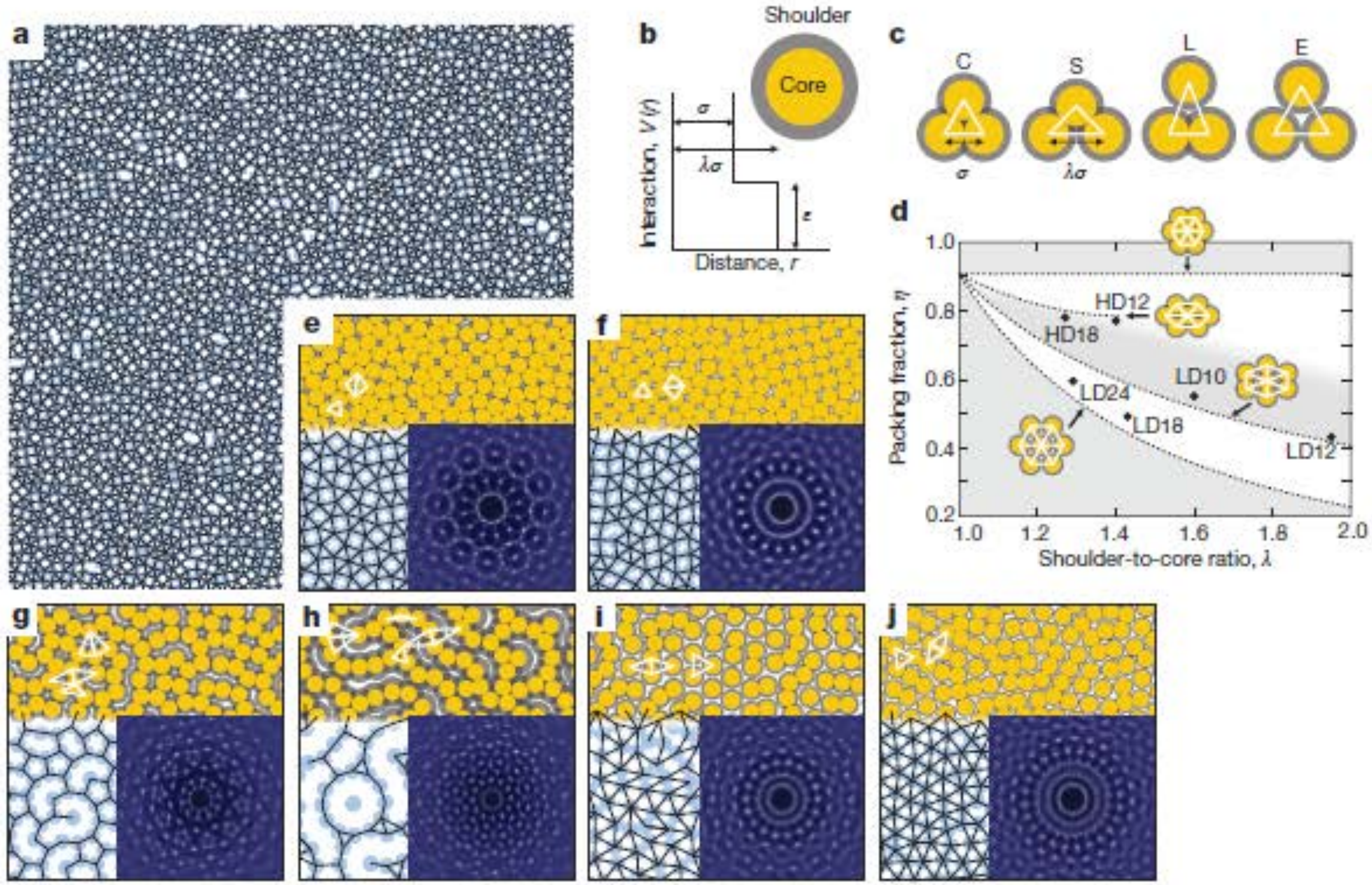


Figure 2: Mosaic two-lengthscale quasicrystals

Nature, Vol 506: 2014, Dotera, Oshiro & Ziherl

In number theory, Riemann zeta function play a crucial role:

$$\begin{aligned}\zeta(s) &= \frac{1}{1^s} + \frac{1}{2^s} + \frac{1}{3^s} + \\ &= (1 + \frac{1}{2^s} + \frac{1}{2^{2s}} + \ldots)(1 + \frac{1}{3^s} + \frac{1}{3^{2s}} + \ldots)(1 + \frac{1}{5^s} + \frac{1}{5^{2s}} + \ldots).\end{aligned}$$

We consider $s = \sigma + \sqrt{-1}t$ to be a complex variable. Then we can formally write:

$$\begin{aligned}\zeta(s) &= 1 + \exp(-s\log 2) + \exp(-s\log 3) + \dots \\ &= \sum_{n=1}^{\infty} \exp(-\sigma\log n - t\log n\sqrt{-1}) \\ &= \sum_{n=1}^{\infty} a_n \exp(2\pi\sqrt{-1}t/\lambda_n)\end{aligned}$$

with $\lambda_n = -2\pi/\log n$. Then $\exp(2\pi t\sqrt{-1}/\lambda_n)$ has a period λ_n. In this way, we may think ζ is a general type of Fourier series:

$$f(t) \sim \sum_{n=0}^{\infty} a_n \exp(2\pi\sqrt{-1}nt).$$

Motivated by Riemann zeta function, Bohr constructed a theory of generalized Fourier expansion, called **almost periodic function**.

A key observation is that such f which is convergent and uniformly bounded are characterized by *almost periodicity*:

For any $\epsilon > 0$ *and there exists* L*'s that* $|f(t)-f(t-L)| < \epsilon$ *for any* t *and such* L *appears with bounded gaps.*

A point set X is **almost periodic** if for any $\varepsilon > 0$ the set of almost period t, that satisfies

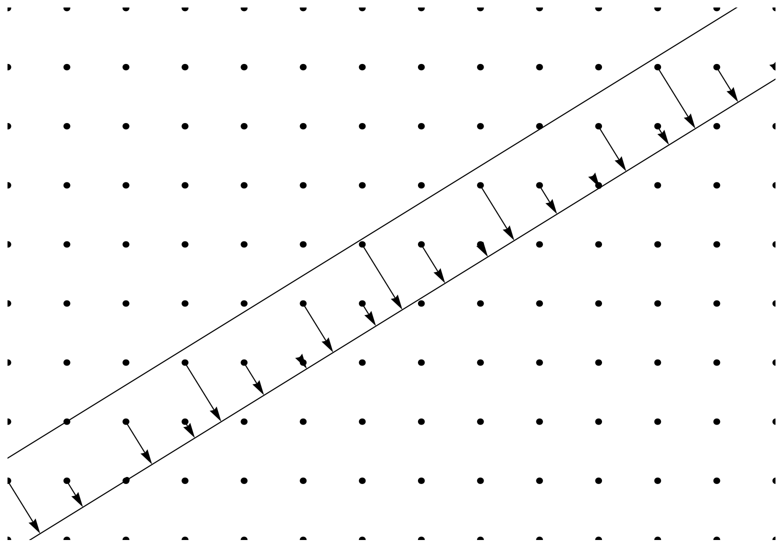
$$\underline{\mathrm{dens}} X \setminus (X - t + B(0, \varepsilon)) < \varepsilon$$

is relatively dense in $\mathbb{R}^d$. Here relatively dense means that t appears with bounded gaps.

This definition is in fact equivalent to pure point diffractiveness of point sets. Thus we may use this as a mathematical definition of quasicrystal.

Almost periodic Delone set is the mathematical model of QC (Baake-Moody[2], Gouéré [4]).

Cut and Project set (Model set) is generated by cut and project scheme, i.e., the set generated by a projection of higher dimensional lattice (LCA group) points stay in some irrational band.



A well known example of aperiodic tiles is due to Penrose which consists of two kinds of tiles: kites and darts with matching rules as in Figure 3:

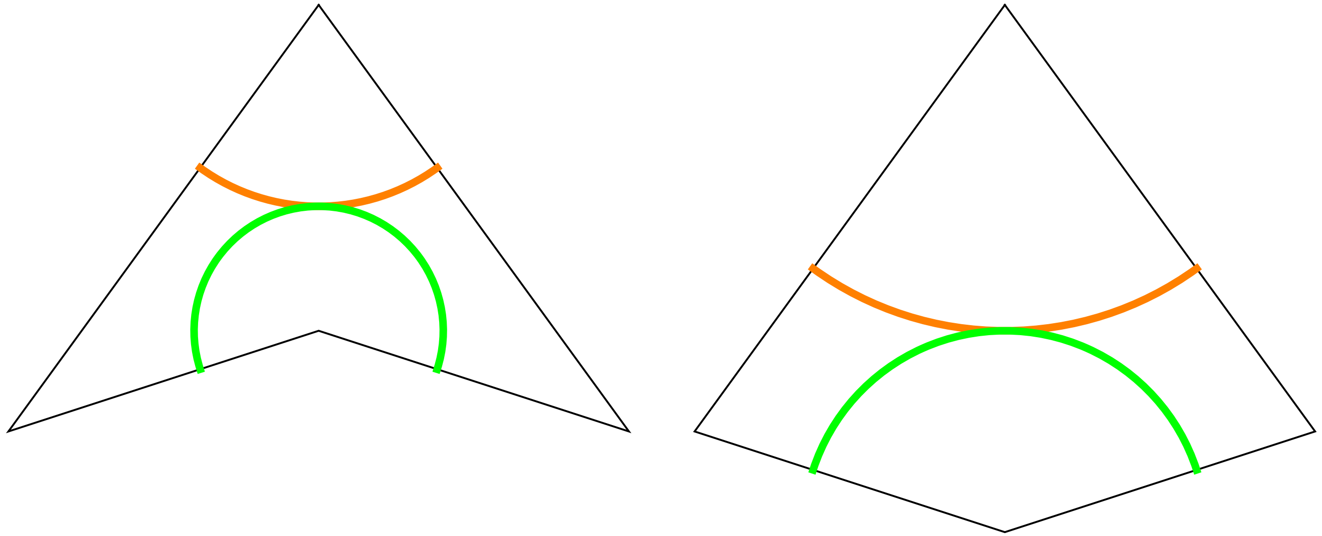


Figure 3: Penrose Tile

that the circular markings must match across the boundary like:

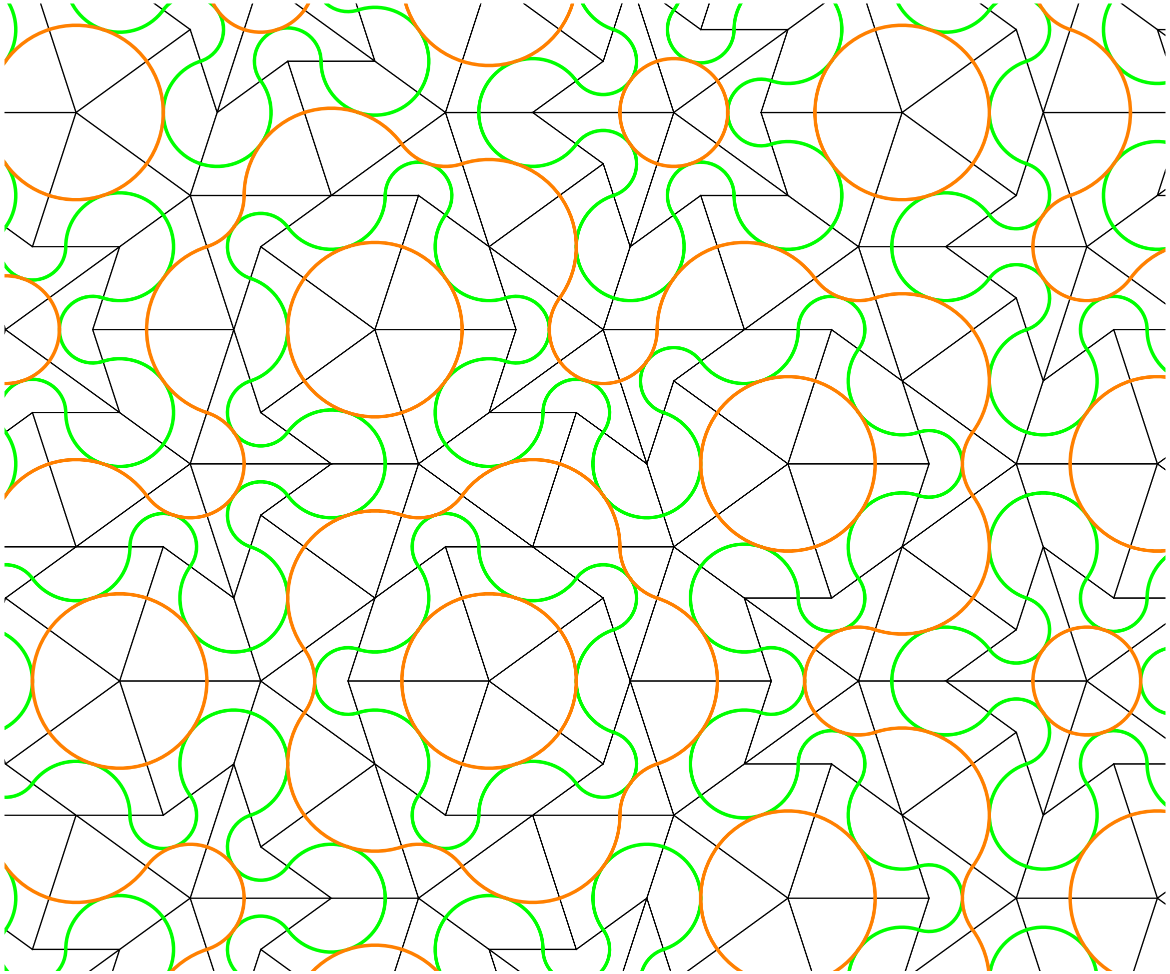


Figure 4: Penrose tiling

To show that Penrose tiles are aperiodic, we have to show two things.

- They admit a tiling.
- Each tiling generated by kite and dart has no period.

de Bruijn [3] showed that Penrose tiling is really a good model of quasi-crystal by showing that its reference point set is understood by **cut and projection**. More precisely such Delone set is the projection of 5-dim lattice points which lies in some irrational band. This assures that the diffraction pattern of Penrose tiling is pure diffractive.

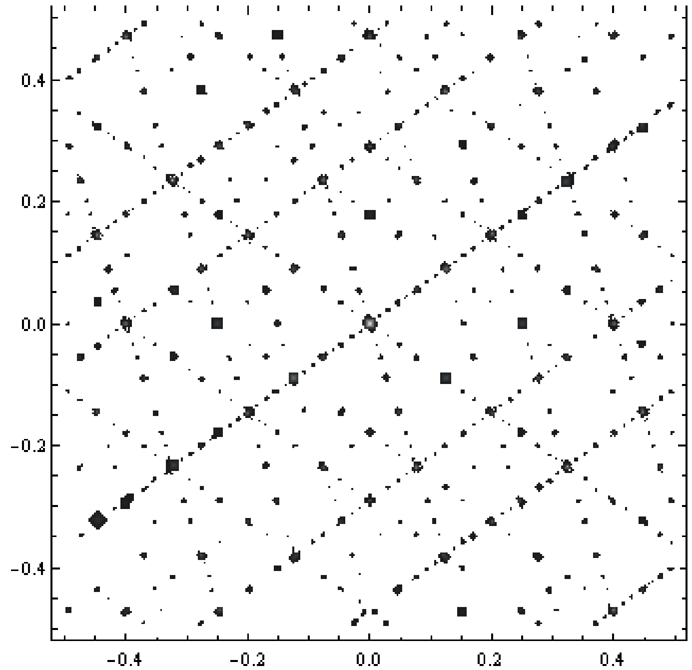


Figure 5: Penrose Diffraction

How can we check that tiling gives a quasicrystal structure ?

Short Answer: Use my Mathematica program to check overlap coincidence.

http://math.tsukuba.ac.jp/~akiyama/Coincidence/Coincidence.html

Self affine tiling is made of prototiles $\mathcal{A} = \{T_1, \ldots, T_m\}$ which satisfies a set equation (substitution rule):

$$QT_j = \bigcup_i T_i + D_{ij}$$

where Q is an expanding matrix and D_{ij} is a finite set of translations.

We use spectral theory of tiling dynamical system. From these data Q and D_{ij} we can check that this gives a quasicrystal structure. Akiyama-J.-Y.Lee [1] gave a practical algorithm on overlap coincidence and implemented into Mathematica program.

Summary

Quasi-crystal is explained better by an aperiodic tile set which produces almost periodic points. For self-affine tilings,

- Bragg peak $\overset{?}{\leftrightarrow}$ Non weak mixing $\iff$ X: Meyer set $\iff$ Q: Pisot family

- Pure pointed diffraction $\iff$ Pure discrete spectrum $\iff$ Overlap Coincidence $\iff$ Cut and projection

- Overlap coincidence can be confirmed by Mathematica.

References

[1] S. Akiyama and J.-Y. Lee, *Algorithm for determining pure pointedness of self-affine tilings*, Adv. Math. **226** (2011), no. 4, 2855–2883.

[2] M. Baake and R.V. Moody, *Weighted dirac combs with pure point diffraction*, J. Reine Angew. Math. **573** (2004), 61–94.

[3] N. G. de Bruijn, *Algebraic theory of Penrose's nonperiodic tilings of the plane. I, II*, Nederl. Akad. Wetensch. Indag. Math. **43** (1981), no. 1, 39–52, 53–66.

[4] J.-B. Gouéré, *Quasicrystals and almost periodicity*, Comm. Math. Phys. **255** (2005), no. 3, 655–681.

[5] D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn, *Metallic phase with long-range orientational order and no translational symmetry*, Phys. Rev. Lett. **53** (1984), no. 20, 1951–1953.