Decagonal quasicrystals

higher dimensional description & structure determination

Hiroyuki Takakura

北海道大学
HOKKAIDO UNIVERSITY

Division of Applied Physics, Faculty of Engineering, Hokkaido University

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Overview

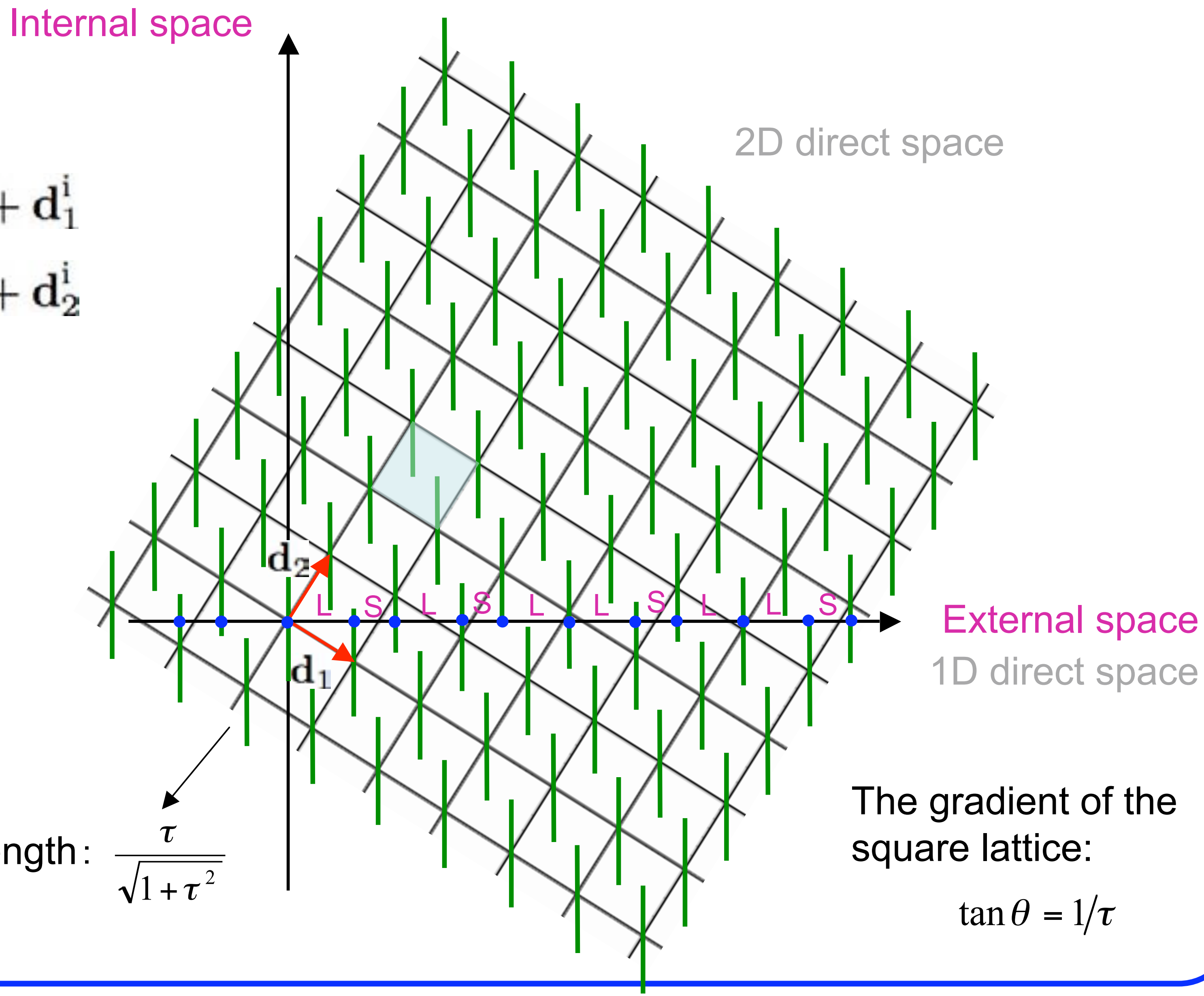
- The section method
- Diffraction symmetry & Space groups of d-QC's
- Unit vectors in decagonal system
- Penrose tiling
- Description of d-QC structures
- Point density
- Simple models
- Symmetry & Space group of d-QC's in a little more details
- Cluster based models
- Example of structure determination of real d-QC's
- Structure factor formula

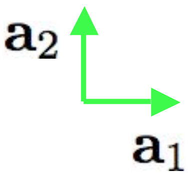
The section method

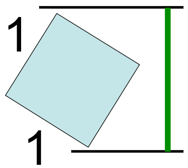
Construction of a Fibonacci sequence

$$\mathbf{d}_1 = \mathbf{d}_1^{e} + \mathbf{d}_1^{i}$$

$$\mathbf{d}_2 = \mathbf{d}_2^{e} + \mathbf{d}_2^{i}$$







Length: $\dfrac{\tau}{\sqrt{1+\tau^2}}$

The gradient of the square lattice:

$$\tan\theta = 1/\tau$$

Diffraction pattern of the Fibonacci sequence

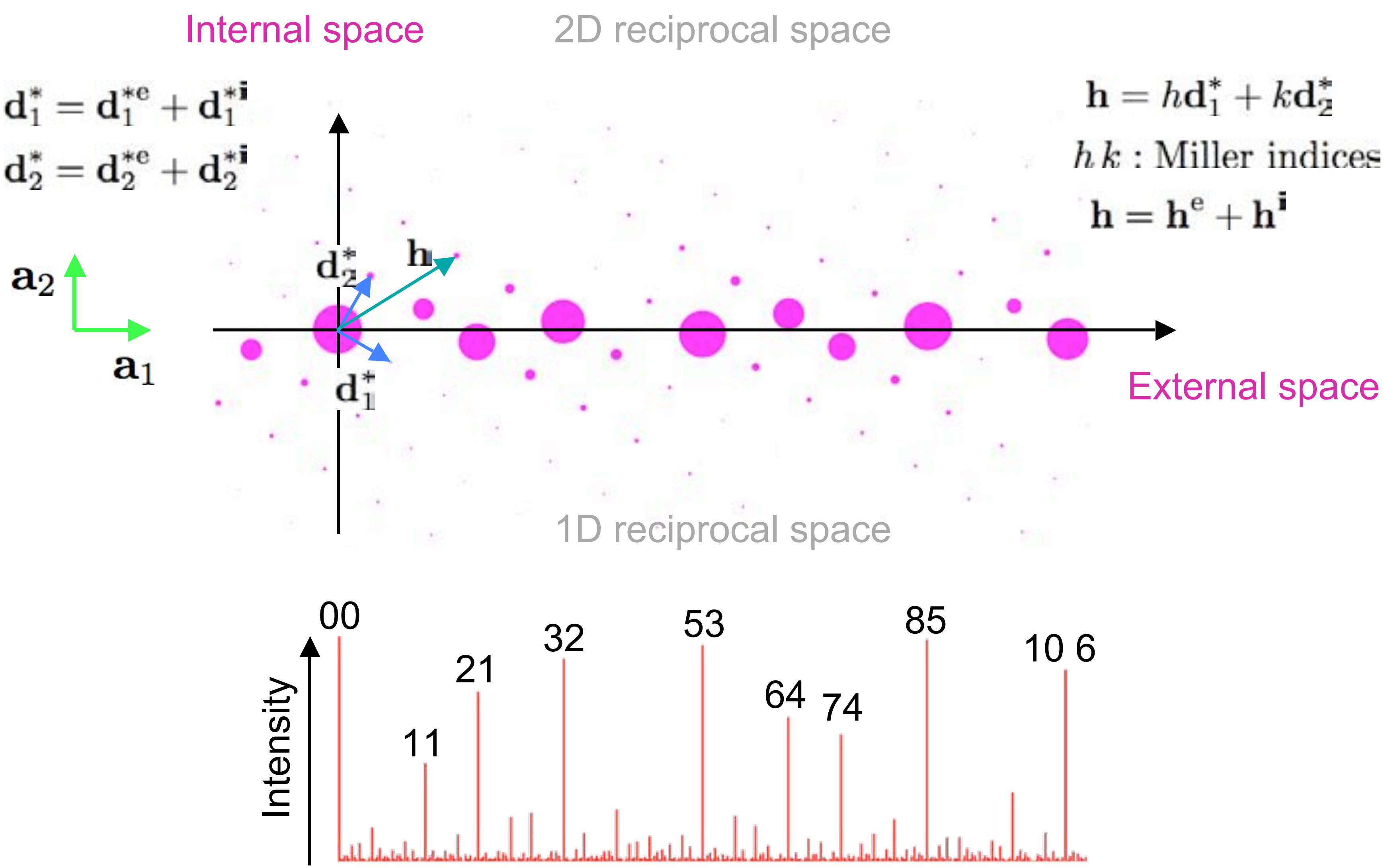
$$\mathbf{d}_1^* = \mathbf{d}_1^{*e} + \mathbf{d}_1^{*i}$$

$$\mathbf{d}_2^* = \mathbf{d}_2^{*e} + \mathbf{d}_2^{*i}$$

$$\mathbf{h} = h\mathbf{d}_1^* + k\mathbf{d}_2^*$$

$h\,k$: Miller indices

$$\mathbf{h} = \mathbf{h}^e + \mathbf{h}^i$$



Direct space

Reciprocal space

Fourier transform

2D crystal

2D reciprocal lattice

Structure

Diffraction pattern

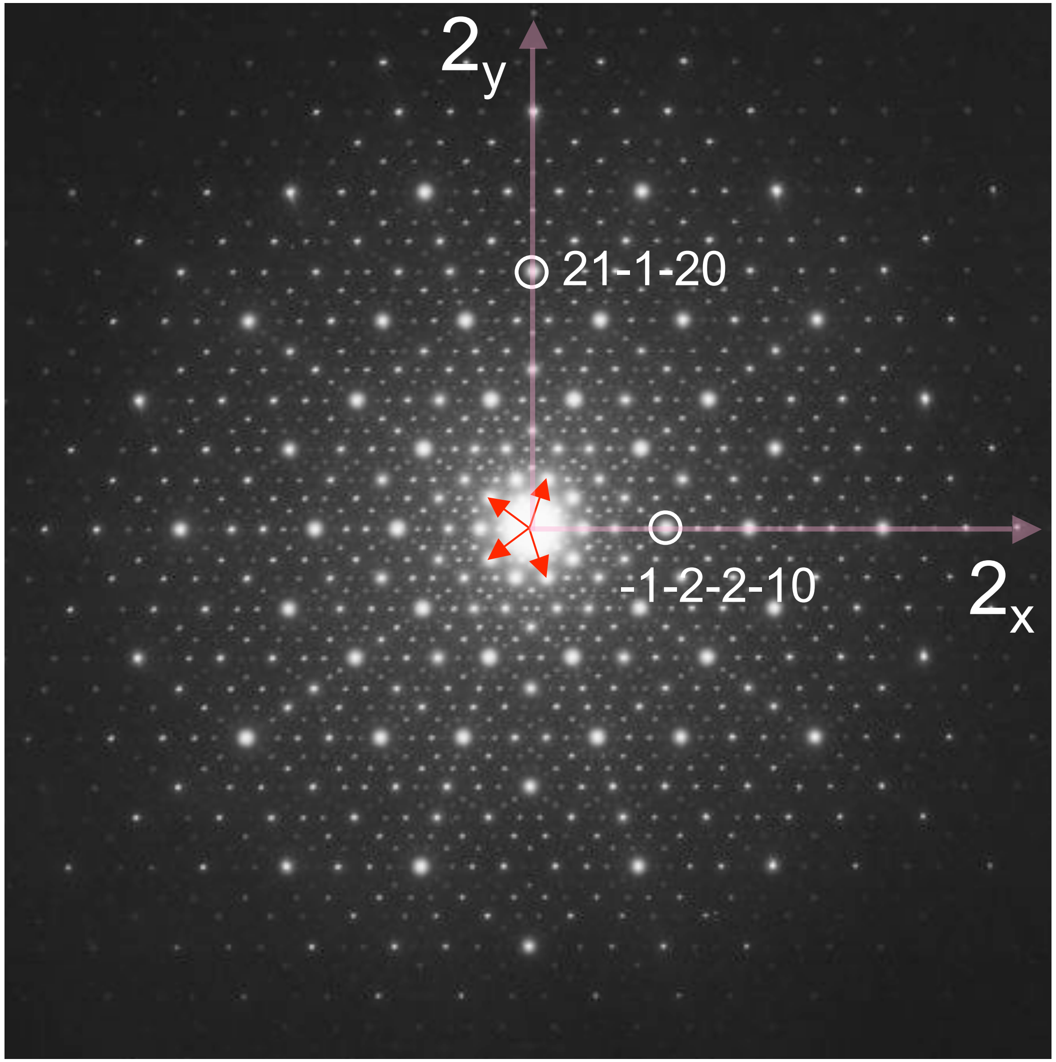
1D section of the 2D crystal

Projection onto 1D along the other 1D.

Fourier transform

Diffraction symmetry
&
Space groups of d-QC's

Diffraction patterns of a decagonal quasicrystal



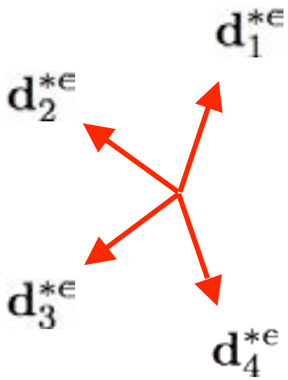
d-$Al_{75.2}Ni_{14.6}Ru_{10.2}$

a = 0.2764 nm

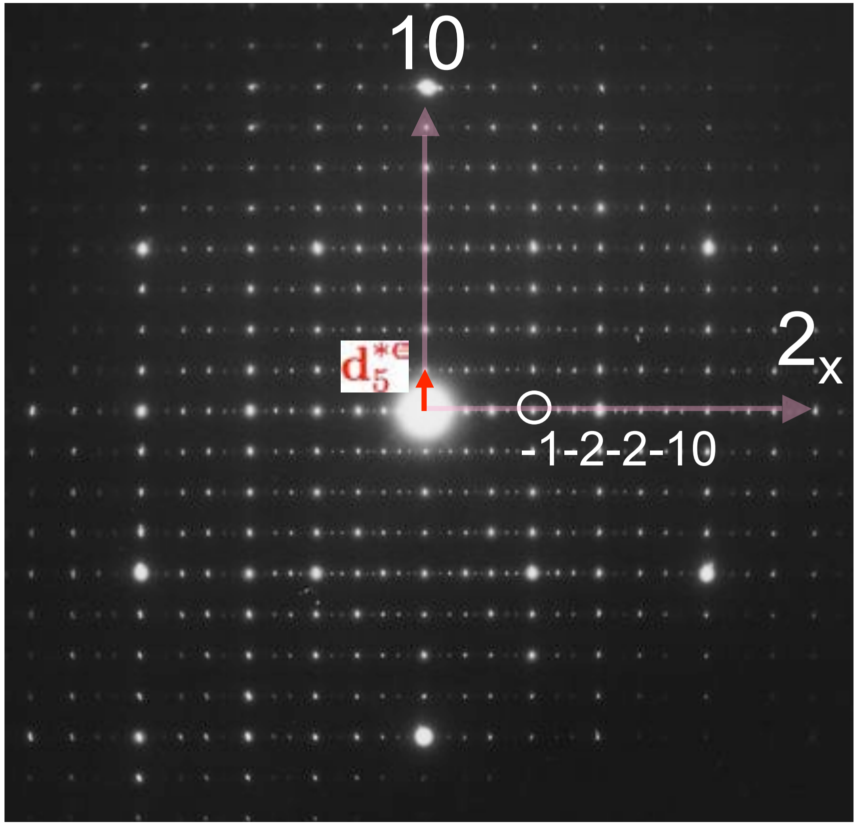
c = 1.6523 nm

$h_1h_2h_3h_40$

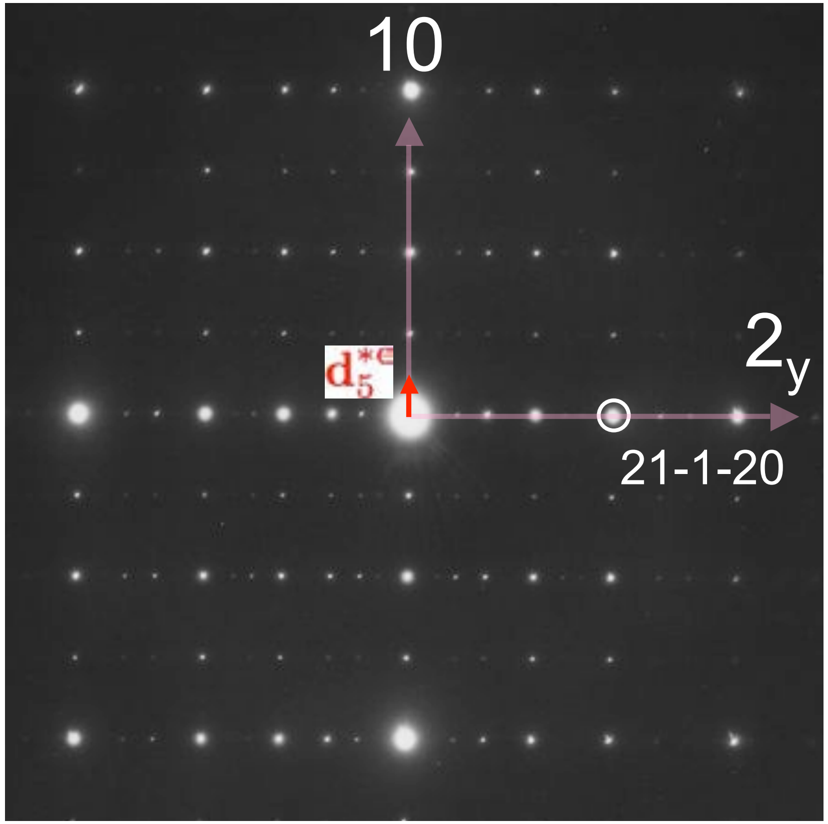
reciprocal lattice plane



$h_1h_2h_2h_1h_5$



$h_1h_2\overline{h}_2\overline{h}_1h_5$

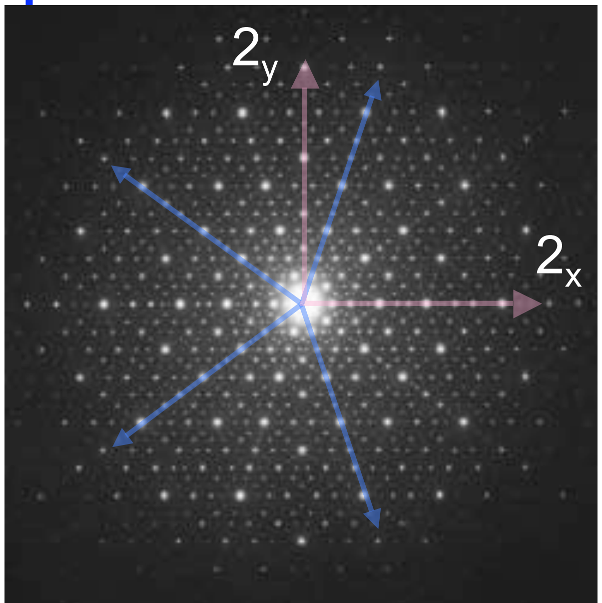


No reflection condition

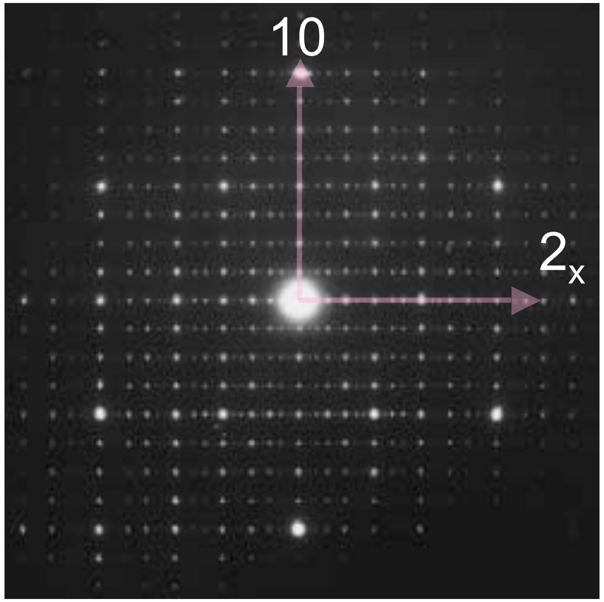
Reflection condition:

$h_5 = 2n$ for $h_1h_2\overline{h}_2\overline{h}_1h_5$

$h_1 h_2 h_3 h_4 0$

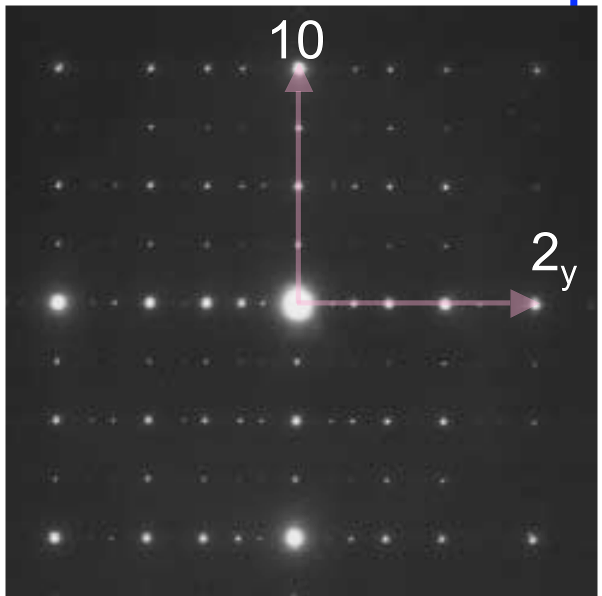


$h_1 h_2 h_2 h_1 h_5$



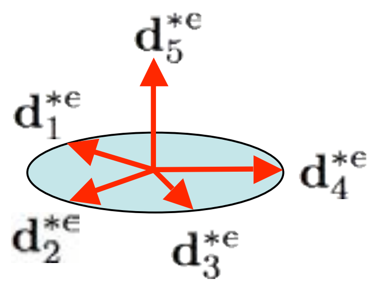
along

$h_1 h_2 \overline{h}_2 \overline{h}_1 h_5$



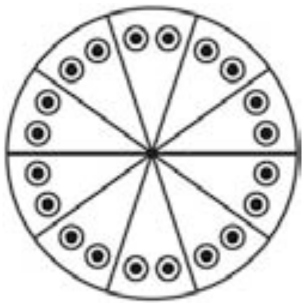
between

All reflections can be indexed with five integer using these unit vectors.



Feature of the diffraction pattern of the d-AlNiRu QC

Diffraction symmetry



$$10/mmm \quad (D_{10h})$$

Order : 40

Rotational symmetry

Reflection condition

$$h_5 = 2n \quad \text{for} \quad h_1 h_2 \bar{h}_2 \bar{h}_1 h_5$$

(Hyper-) glide plane

$$\{\sigma' | \mathbf{t}(\sigma')\}$$

Non-primitive translation vector

Decagonal space groups in 5D space with highest symmetries

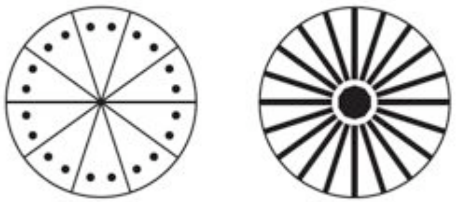
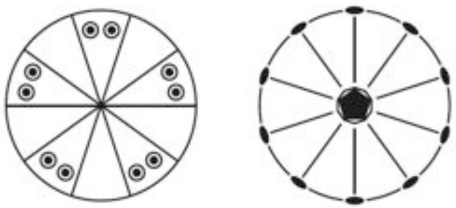
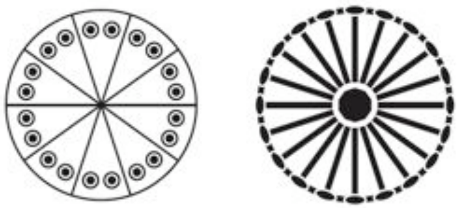
Point group	Space group	Special reflection condition	
10/mmm*	$P10/mmm$	No condition	
	$P10/mcc$	$h_5 = 2n$ for $h_1h_2h_2h_1h_5$ $h_5 = 2n$ for $h_1h_2\bar{h}_2\bar{h}_1h_5$	along between
	$\boxed{P10_5/mmc}$	$\boxed{h_5 = 2n \text{ for } h_1h_2\bar{h}_2\bar{h}_1h_5}$	between
	$P10_5/mcm$	$h_5 = 2n$ for $h_1h_2h_2h_1h_5$	along

* The order of the point group is 40.

There are 34 decagonal non-equivalent space groups.

Cf. D.A.Rabson *et al.*, *Rev. Mod. Phys.* **63** (1990) 699-733.

Possible space groups of the d-AlNiRu QC

Order		Point group	Space group	
20		$10mm$ (C_{10v})	$P10_5mc$	○
20		$\overline{10}m2$ (D_{5h})	$P\overline{10}m2$	×
40		$10/mmm$ (D_{10h})	$P10_5/mmc$	○

What to Remember

Diffraction patterns of d-QC's can be indexed with five integers.

→ Reciprocal lattice in 5D space

↓

Crystal in 5D space

Unit vectors in decagonal system

A flowchart representing a process for determining the unit vectors of d-QC's

Point group symmetry

Diffraction pattern

$\downarrow \ \mathbf{d}_i^{*\mathrm{e}}$

Special reflection conditions (Extinction rules)

5D reciprocal lattice

Indexing

5 indices: $h_1 \ h_2 \ h_3 \ h_4 \ h_5$

Lattice constants: a^*, c^*

$\downarrow$

Unit vectors in 5D reciprocal space

$$\mathbf{d}_i^* = \sum_{j=1}^{5} \tilde{M}_{ij}^{-1} \mathbf{a}_j$$

$$\mathbf{d}_i^* = \mathbf{d}_i^{*\mathrm{e}} + \mathbf{d}_i^{*\mathrm{i}}$$

$\downarrow$

Unit vectors in 5D direct space

$$\mathbf{d}_i = \sum_{j=1}^{5} M_{ij} \mathbf{a}_j$$

$$\mathbf{d}_i = \mathbf{d}_i^{\mathrm{e}} + \mathbf{d}_i^{\mathrm{i}}$$

Unit vectors in 5D reciprocal space

$\mathbf{d}_i^* \ (i = 1, 2, \ldots, 5)$: unit reciprocal lattice vectors

$\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4, \mathbf{a}_5$: orthonormal base vectors

$\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_5$: external (3D)

$\mathbf{a}_3, \mathbf{a}_4$: internal (2D)

($\mathbf{a}_1, \mathbf{a}_2$ for 2D quasiperiodic plane)

$$\mathbf{d}_i^* = \sum_{j=1}^{5} \tilde{M}_{ij}^{-1} \mathbf{a}_j$$

$$\tilde{M}^{-1} = \frac{a^*}{\sqrt{5}} \begin{pmatrix} c_1 & s_1 & c_2 & s_2 & 0 \\ c_2 & s_2 & c_4 & s_4 & 0 \\ c_3 & s_3 & c_1 & s_1 & 0 \\ c_4 & s_4 & c_3 & s_3 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{5}c^*/a^* \end{pmatrix}$$

$a^* = a^{*\mathrm{e}} = a^{*\mathrm{i}}$

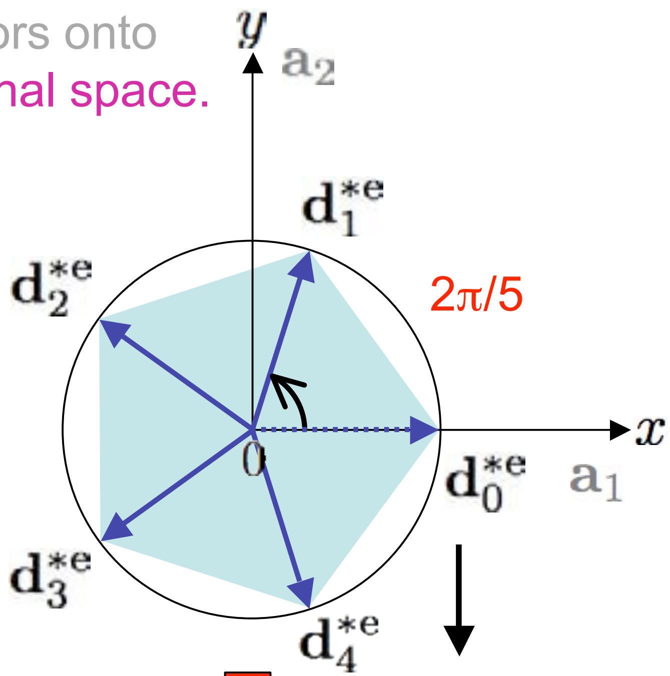
$c_j = \cos(2\pi j/5), \ s_j = \sin(2\pi j/5)$

$(j = 1, 2, \ldots, 5)$

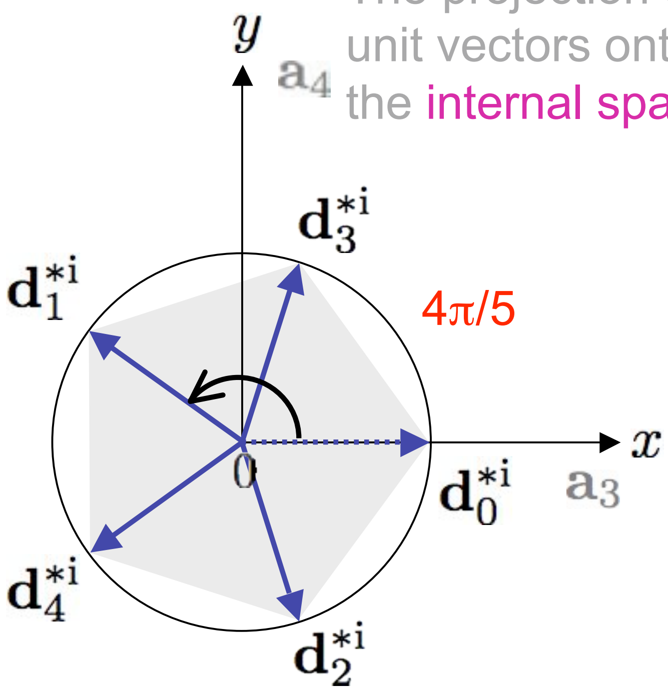
a^*, c^* : lattice constants

Projections of the unit vectors $\mathbf{d}_i^*$

The projection of the unit vectors onto the external space.



The projection of the unit vectors onto the internal space.



$$\mathbf{d}_0^{*e} = -\mathbf{d}_1^{*e} - \mathbf{d}_2^{*e} - \mathbf{d}_3^{*e} - \mathbf{d}_4^{*e}$$

For Indexing

$$\mathbf{d}_i^{*e} = \frac{a^*}{\sqrt{5}}[c_i\mathbf{a}_1 + s_i\mathbf{a}_2] \quad i = 1,2,3,4$$

$$\mathbf{d}_i^{*i} = \frac{a^*}{\sqrt{5}}[c_{2i}\mathbf{a}_3 + s_{2i}\mathbf{a}_4] \quad i = 1,2,3,4$$

Unit vectors in 5D direct space

Reciprocal lattice vectors → Direct lattice vectors

$$\mathbf{d}_i^* \ (i=1,2,\ldots,5) \rightarrow \mathbf{d}_i \ (i=1,2,\ldots,5)$$

$$\boxed{\mathbf{d}_i = \sum_{j=1}^{5} M_{ij}\mathbf{a}_j}$$

$$M = \frac{2a}{\sqrt{5}} \begin{pmatrix} c_1-1 & s_1 & c_2-1 & s_2 & 0 \\ c_2-1 & s_2 & c_4-1 & s_4 & 0 \\ c_3-1 & s_3 & c_1-1 & s_1 & 0 \\ c_4-1 & s_4 & c_3-1 & s_3 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{5}c/(2a) \end{pmatrix}$$

$$c_j = \cos(2\pi j/5), \ s_j = \sin(2\pi j/5)$$

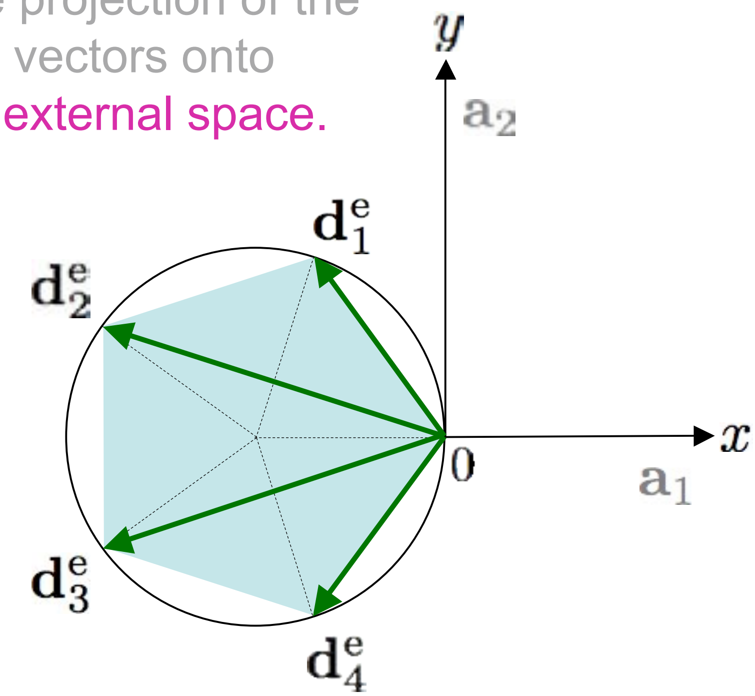
$(j=1,2,3,4)$

$a, \ c$: lattice constants

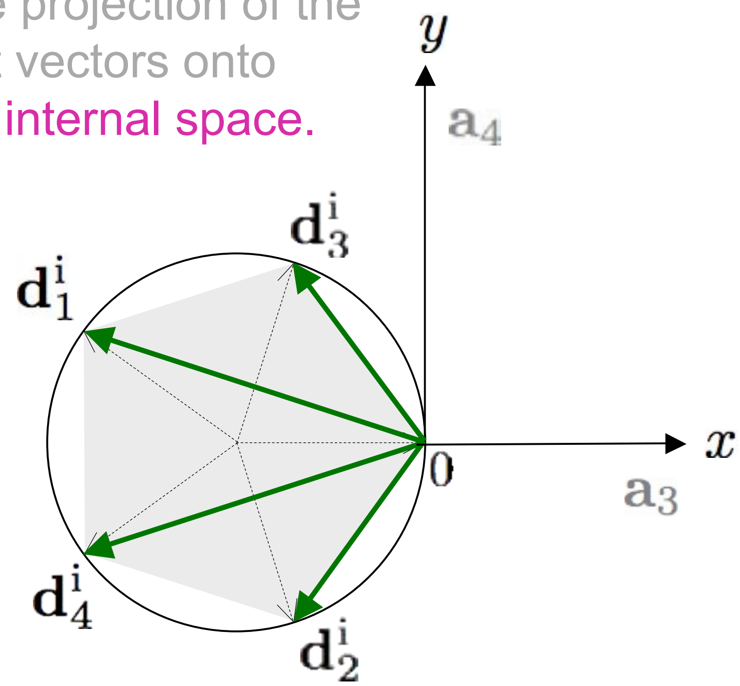
$$a = 1/a^*, \ c = 1/c^*$$

Projections of the unit vectors $\mathbf{d}_i$

The projection of the unit vectors onto the external space.



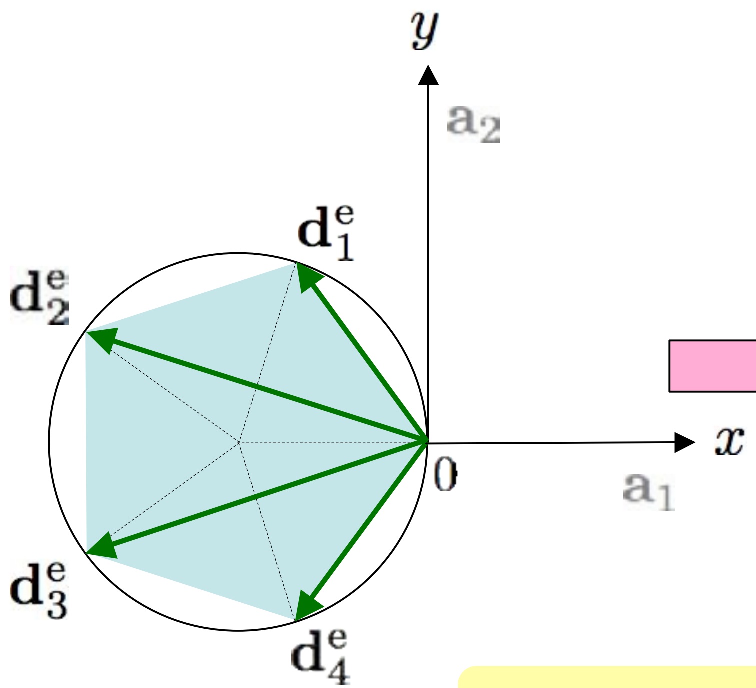
The projection of the unit vectors onto the internal space.

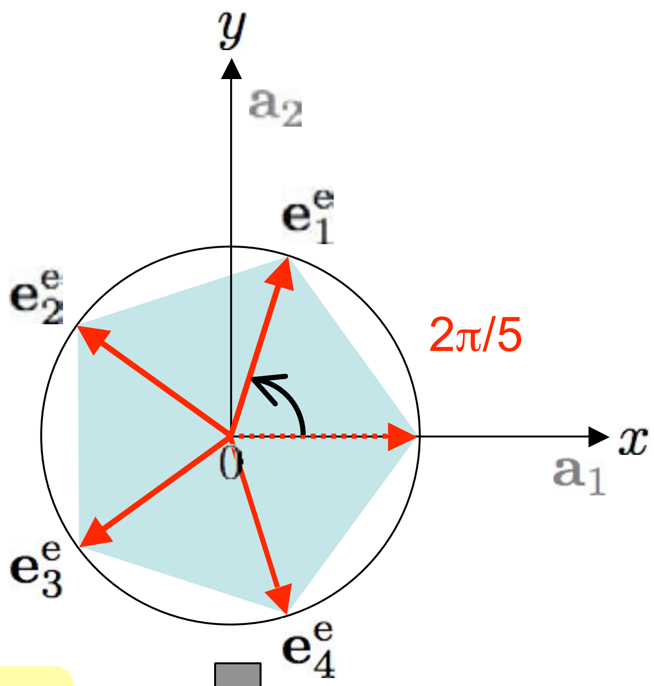


$$\mathbf{d}_i^{\mathrm{e}} = \frac{2a}{\sqrt{5}}[(c_i - 1)\mathbf{a}_1 + s_i\mathbf{a}_2] \qquad i = 1, 2, 3, 4$$

$$\mathbf{d}_i^{\mathrm{i}} = \frac{2a}{\sqrt{5}}[(c_{2i} - 1)\mathbf{a}_3 + s_{2i}\mathbf{a}_4] \qquad i = 1, 2, 3, 4$$

Vectors for specifying atom positions in the 2D external space





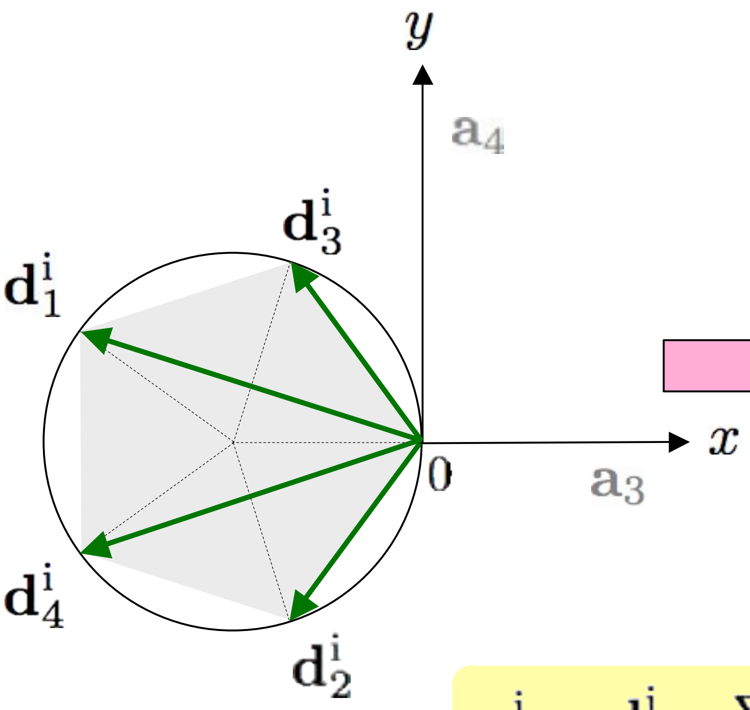
$$\mathbf{e}_i^{\mathrm{e}} = \mathbf{d}_i^{\mathrm{e}} - \sum_{l=1}^{4} \mathbf{d}_l^{\mathrm{e}}/5$$

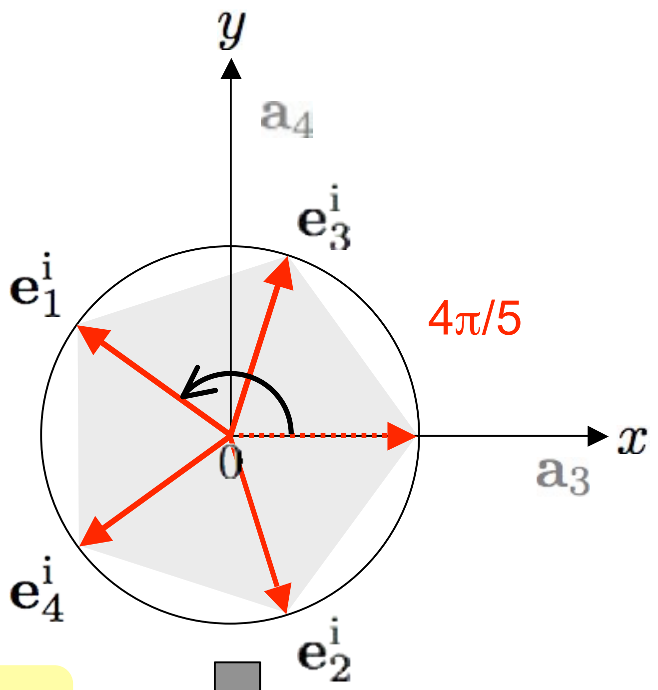
$$\mathbf{d}_i^{\mathrm{e}} = \frac{2a}{\sqrt{5}}[(c_i - 1)\mathbf{a}_1 + s_i\mathbf{a}_2]$$

$$i = 1, 2, 3, 4$$

$$\boxed{\mathbf{e}_i^{\mathrm{e}} = \frac{2a}{\sqrt{5}}[c_i\mathbf{a}_1 + s_i\mathbf{a}_2] \quad i = 1, 2, 3, 4}$$

Vectors employed for defining occupation domains in the internal space





$$\mathbf{e}^{\mathrm{i}}_i = \mathbf{d}^{\mathrm{i}}_i - \sum_{l=1}^{4} \mathbf{d}^{\mathrm{i}}_l/5$$

$$\mathbf{d}^{\mathrm{i}}_i = \frac{2a}{\sqrt{5}}[(c_{2i}-1)\mathbf{a}_3 + s_{2i}\mathbf{a}_4]$$

$$i = 1, 2, 3, 4$$

$$\mathbf{e}^{\mathrm{i}}_i = \frac{2a}{\sqrt{5}}[c_{2i}\mathbf{a}_3 + s_{2i}\mathbf{a}_4]$$

$$i = 1, 2, 3, 4$$

Similarity transformation

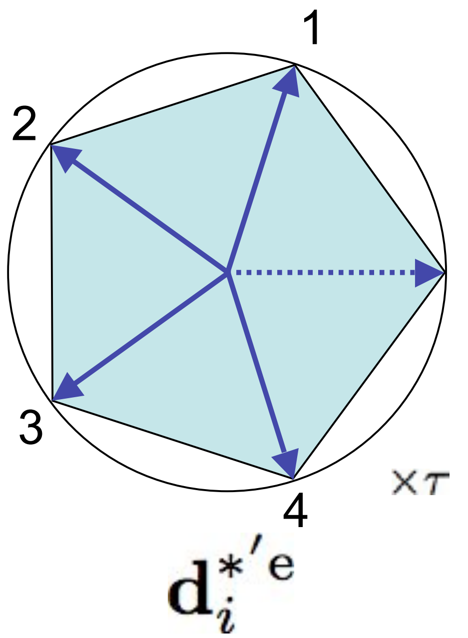
Choice of $\mathbf{d}_i^*$ is not unique.

$$\mathbf{d}_i^{*'} = \sum_{j=1}^{5} [(\tilde{S})^m]_{ij} \mathbf{d}_j^*$$

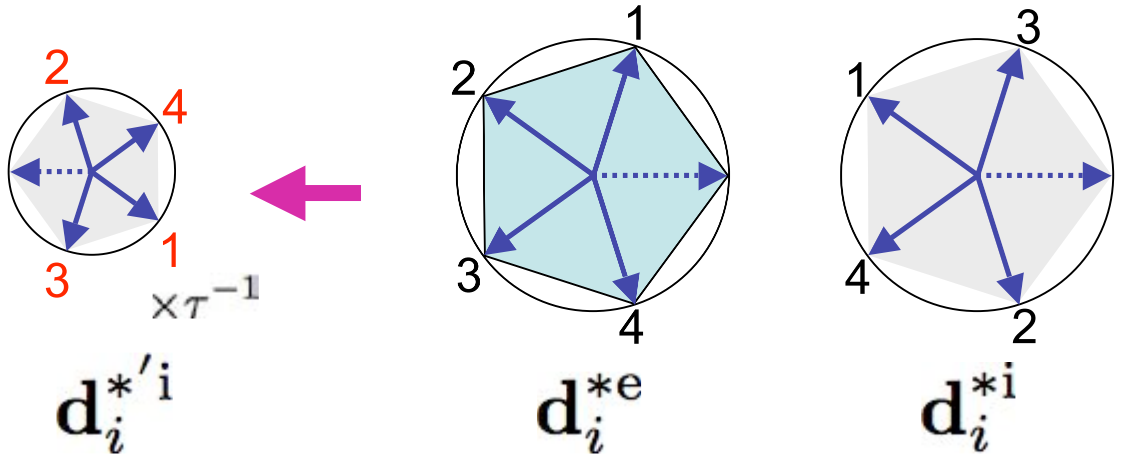
$$S = \begin{bmatrix} 0 & 1 & 0 & -1 & 0 \\ 0 & 1 & 1 & -1 & 0 \\ -1 & 1 & 1 & 0 & 0 \\ -1 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\det(S) = 1$$

$\tilde{S}$: transposed matrix of S

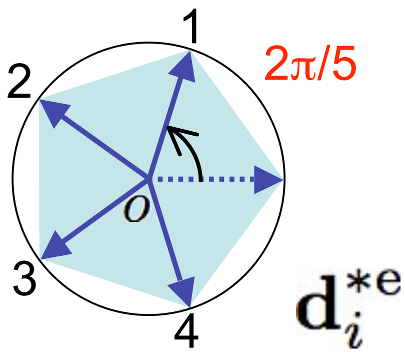


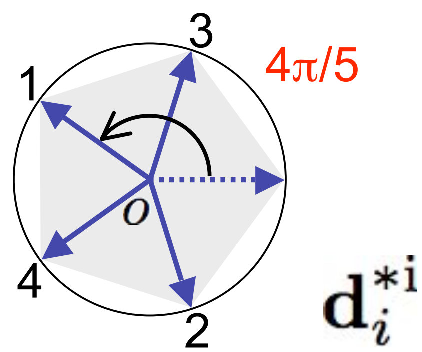
The case $m = 1$



What to Remember

External space | Internal space

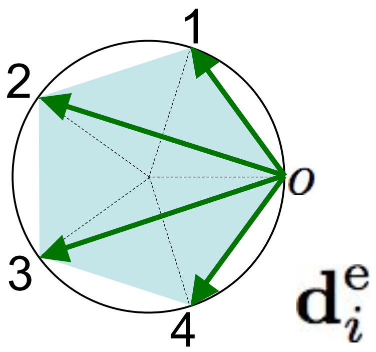


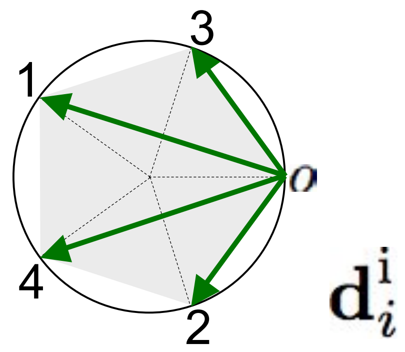


Reciprocal space

$$\mathbf{d}_i^{*} = \mathbf{d}_i^{*\mathrm{e}} + \mathbf{d}_i^{*\mathrm{i}}$$

$$i = 1, 2, 3, 4$$

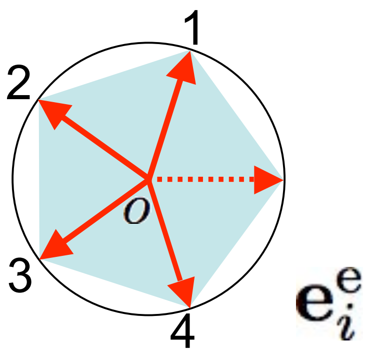


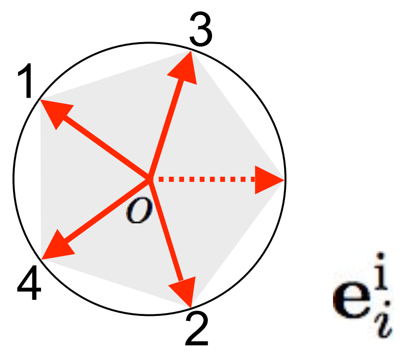


Direct space

$$\mathbf{d}_i = \mathbf{d}_i^{\mathrm{e}} + \mathbf{d}_i^{\mathrm{i}}$$

$$i = 1, 2, 3, 4$$





$$\mathbf{e}_i^{\mathrm{e}} = \mathbf{d}_i^{\mathrm{e}} - \sum_{l=1}^{4} \mathbf{d}_l^{\mathrm{e}}/5$$

$$\mathbf{e}_i^{\mathrm{i}} = \mathbf{d}_i^{\mathrm{i}} - \sum_{l=1}^{4} \mathbf{d}_l^{\mathrm{i}}/5$$

$$i = 1, 2, 3, 4$$

- The first four vectors, $\mathbf{d}_i^* \ (i = 1, 2, 3, 4)$, are relevant to the quasi-periodic plane of d-QC.
- Choice of a^* is not unique.
- A similarity transformation does not change the size of the 5D unit cell, but changes the scale of the projected vectors in the external and internal spaces.

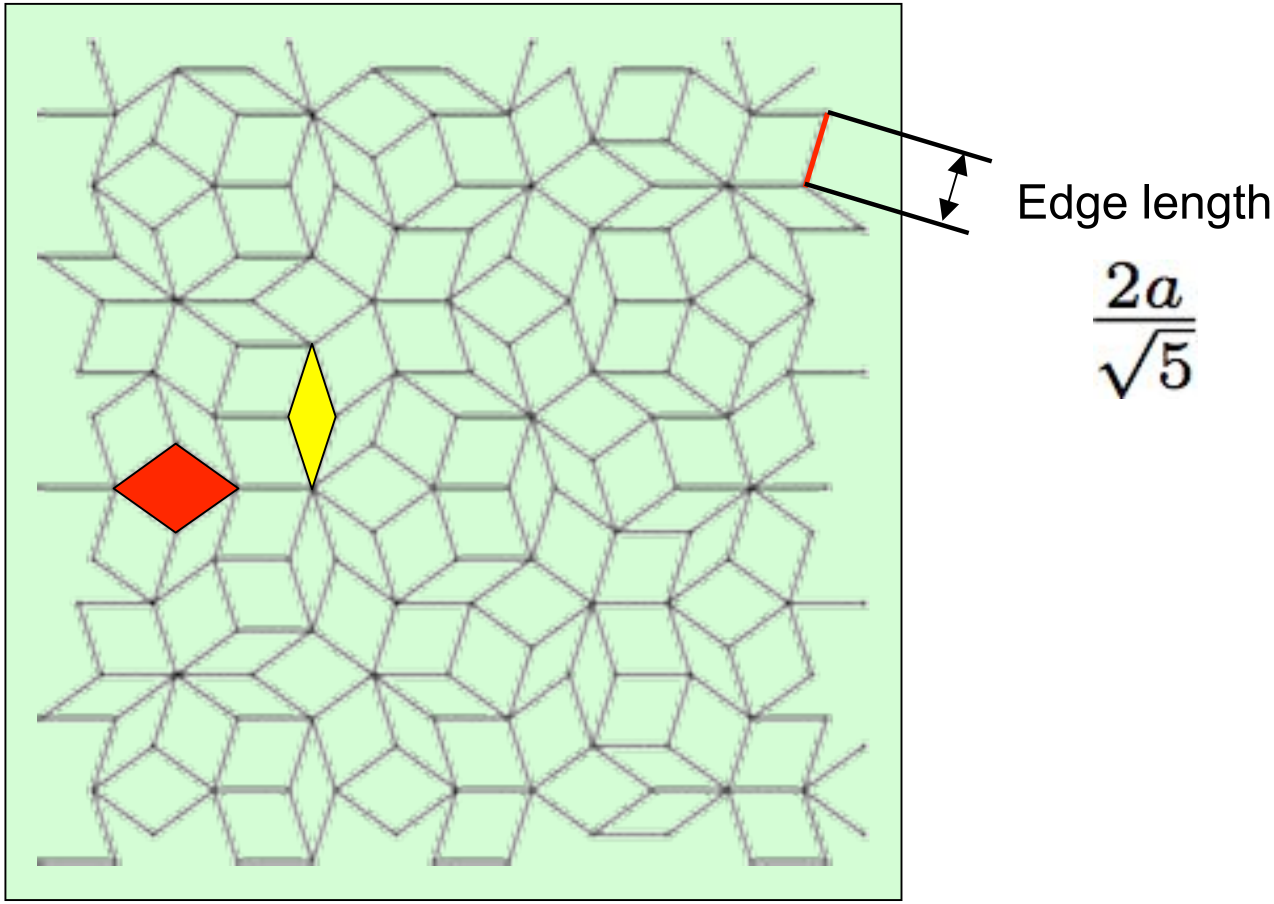
Description of d-QC structures

D-QC structure

- Periodic stacking of atom planes along the 10-fold axis.
- Each plane has a quasiperiodic atomic order.

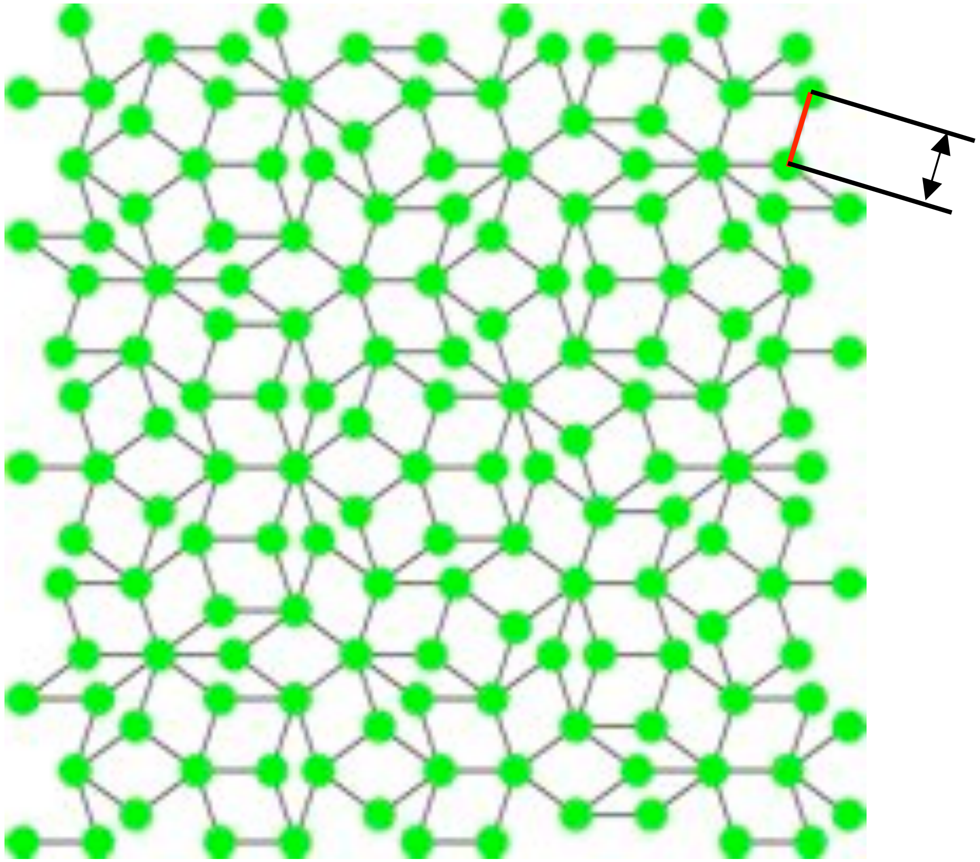
→ A decorated Penrose tiling with atoms would give an example of such atomic plane.

Penrose tiling



$$\frac{2a}{\sqrt{5}}$$

Decoration of the Penrose tiling with atoms

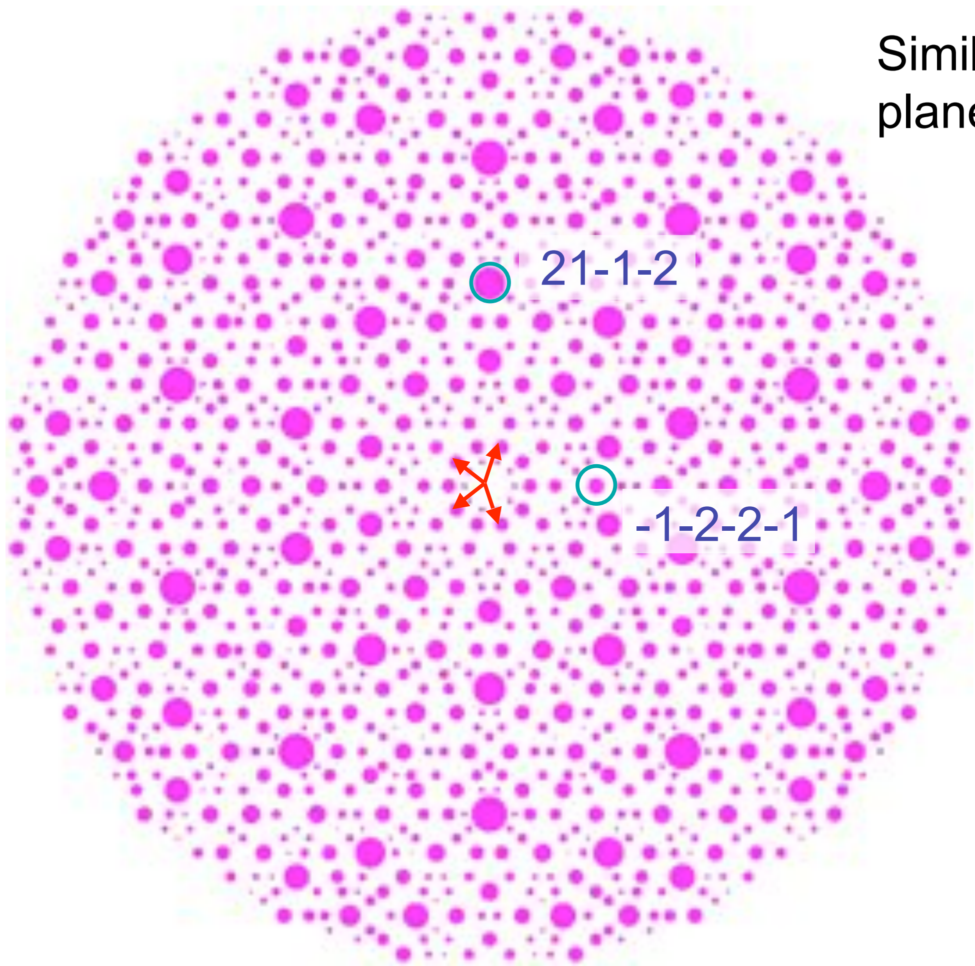


Edge length

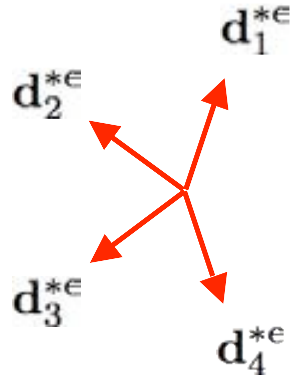
$$\frac{2a}{\sqrt{5}}$$

Vertex decoration

Diffraction pattern of the Penrose tiling



Similar to $h_1h_2h_3h_40$ plane of real d-QC

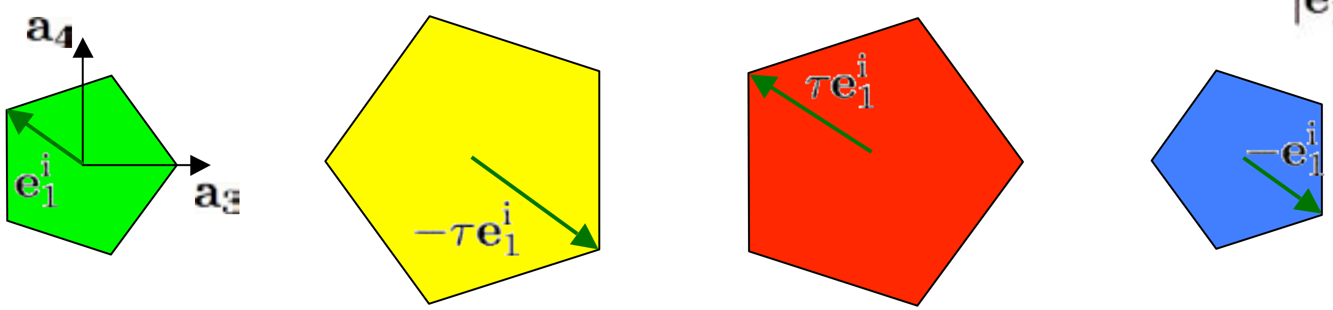


Vertex decoration with point scatters

Construction of the Penrose tiling

Occupation domains:

$$|\mathbf{e}_1^{\mathrm{i}}| = \frac{2a}{\sqrt{5}}$$



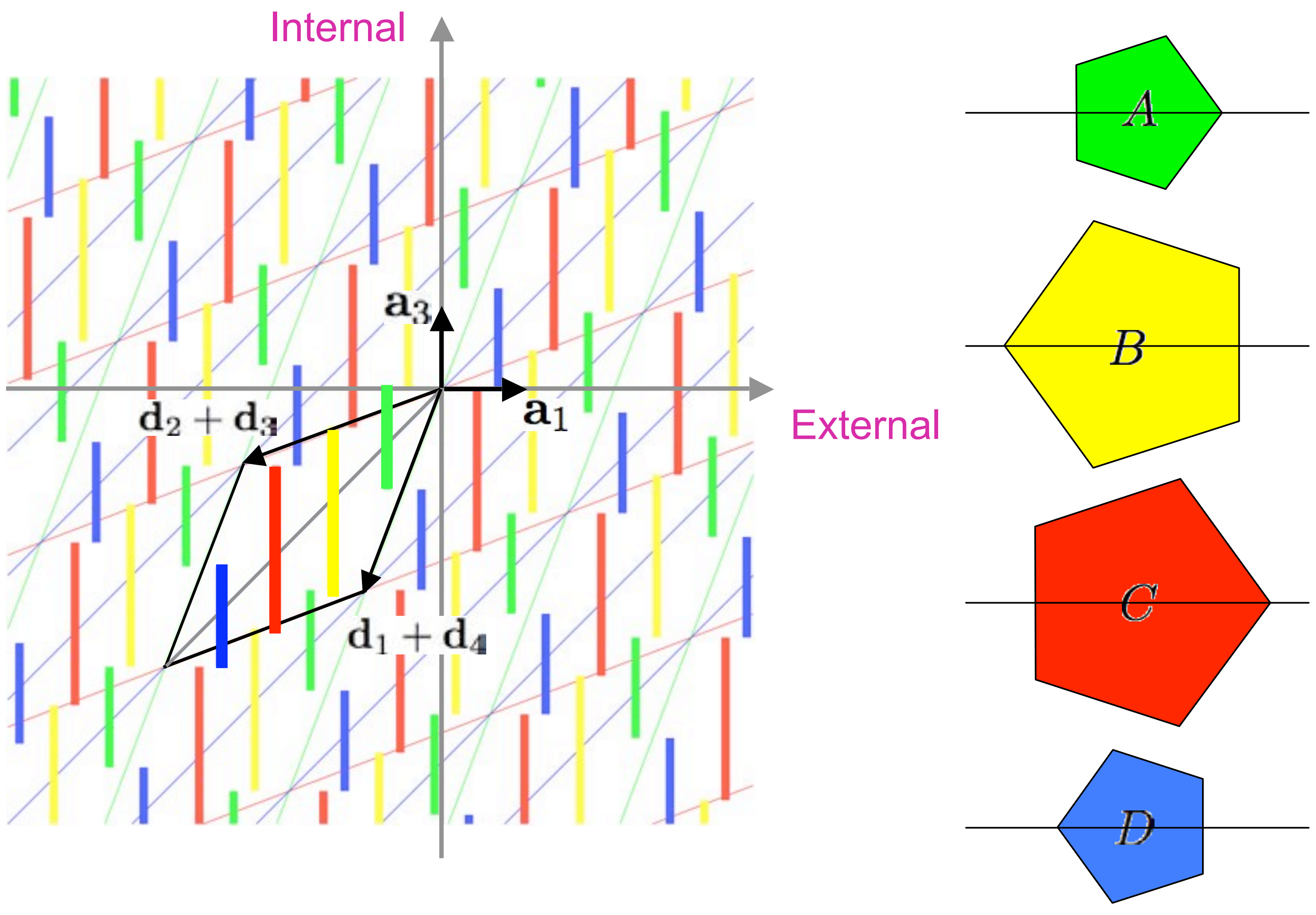
A	B	C	D
$(\frac{1}{5},\frac{1}{5},\frac{1}{5},\frac{1}{5})$	$(\frac{2}{5},\frac{2}{5},\frac{2}{5},\frac{2}{5})$	$(\frac{3}{5},\frac{3}{5},\frac{3}{5},\frac{3}{5})$	$(\frac{4}{5},\frac{4}{5},\frac{4}{5},\frac{4}{5})$

The 4D unit cell: $\mathbf{d}_i \ (i = 1, 2, 3, 4)$

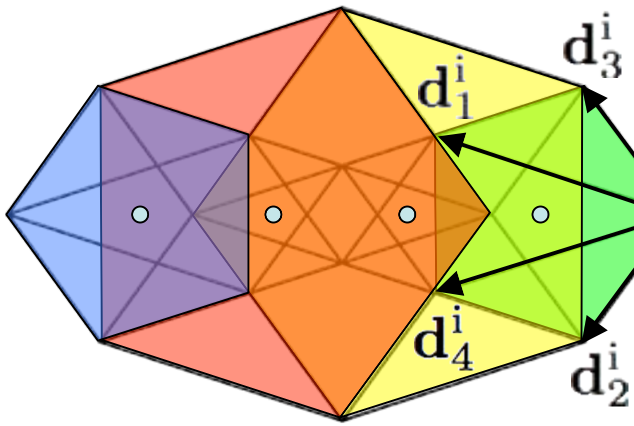
Lattice constant: a

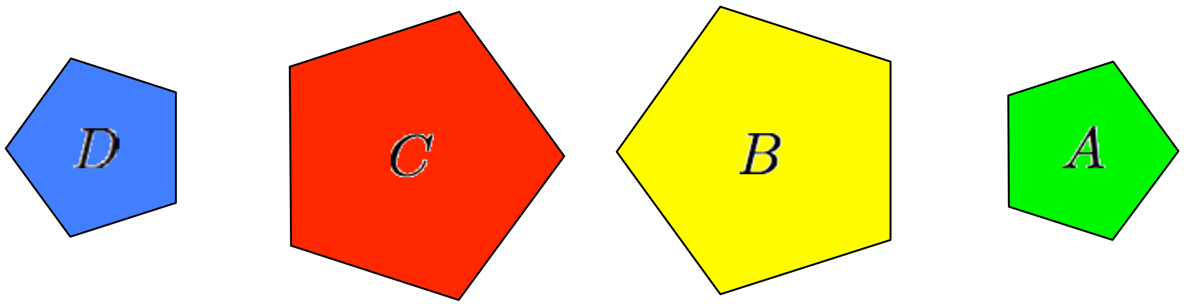
$$\mathbf{e}_i^{\mathrm{i}} = \frac{2a}{\sqrt{5}}[c_{2i}\mathbf{a}_3 + s_{2i}\mathbf{a}_4] \qquad i = 1, 2, 3, 4$$

2D section of 4D structure



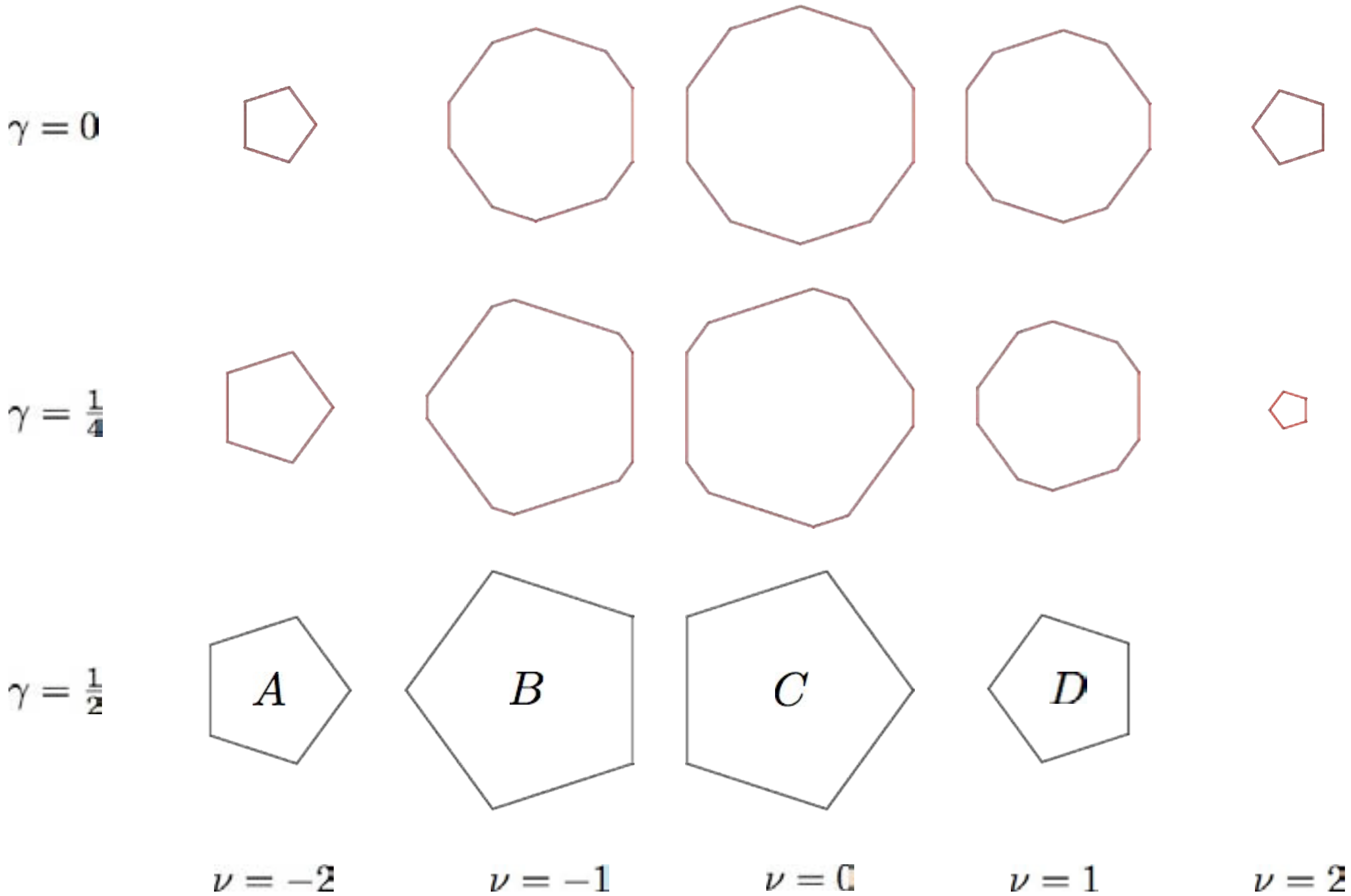
Projection of the 4D unit cell onto the 2D internal space





$(\frac{4}{5},\frac{4}{5},\frac{4}{5},\frac{4}{5})$ $(\frac{3}{5},\frac{3}{5},\frac{3}{5},\frac{3}{5})$ $(\frac{2}{5},\frac{2}{5},\frac{2}{5},\frac{2}{5})$ $(\frac{1}{5},\frac{1}{5},\frac{1}{5},\frac{1}{5})$

Generalized Penrose tiling



Point density

- The point density is the number of vertices per unit area (or volume) of a tiling.
- Because the density of QC's is a fundamental quantity, therefore it has to be explained by their models.

- The density calculations are based on the fact that an OD at some lattice point n intersects the external space at a point and the set of all possible cross points covers the OD homogeneously.

Point density calculation

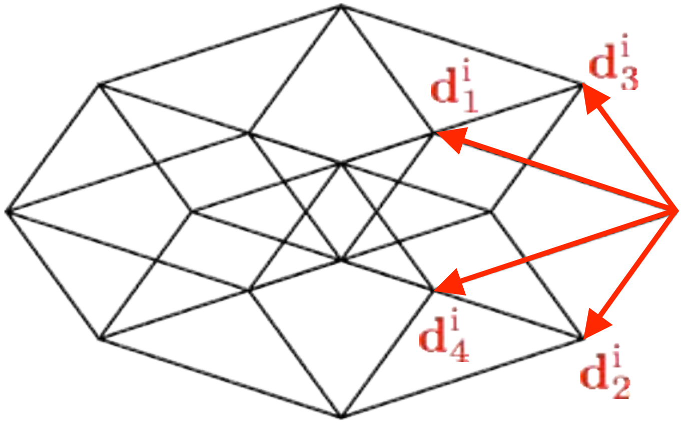
Unit vectors of the nD lattice: $\mathbf{d}_i = \sum_{j=1}^{n} M_{ij}\mathbf{a}_i$

The unit-cell volume: $\Omega_0 = \det|M|$

Sum of the area (volume) of the OD's : Ω^{i}

Point density: $\rho_{\mathrm{pd}} = \Omega^{\mathrm{i}}/\Omega_0$

Point density of the primitive 4D decagonal lattice



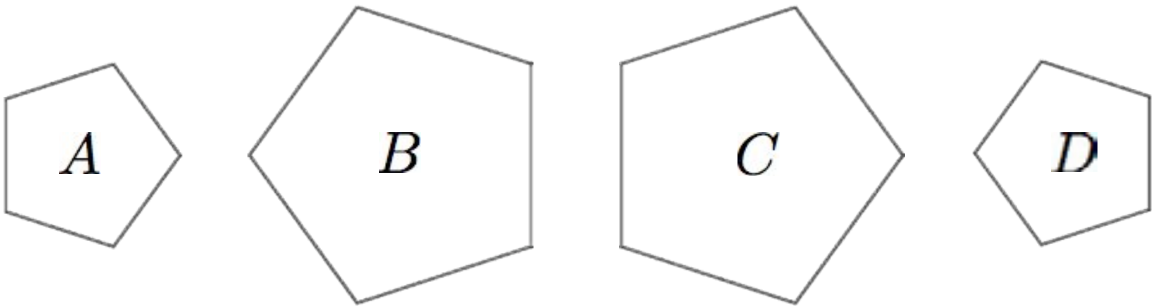
Primitive 4-dimensional decagonal lattice: $\mathbf{d}_j \ (j = 1, 2, 3, 4)$

The unit-cell volume: $\Omega_0 = \det|M| = 4\sqrt{5}a^4$

Area of the unit cell in the internal space: $\Omega_0^{\mathrm{i}} = 4\tau^3 \sin(\pi/5)a^2$

Point density: $\rho_0 = \Omega_0^{\mathrm{i}}/\Omega_0 = \tau^3 \sin(\pi/5)/(\sqrt{5}a^2)$

Point density of the Penrose tiling



$\nu = 1$ $\nu = 2$ $\nu = 3$ $\nu = 4$

Point density ρ_{pd} $\propto$ Area of the occupation domains $\sum_\nu \Omega^{\mathrm{i}}_\nu$

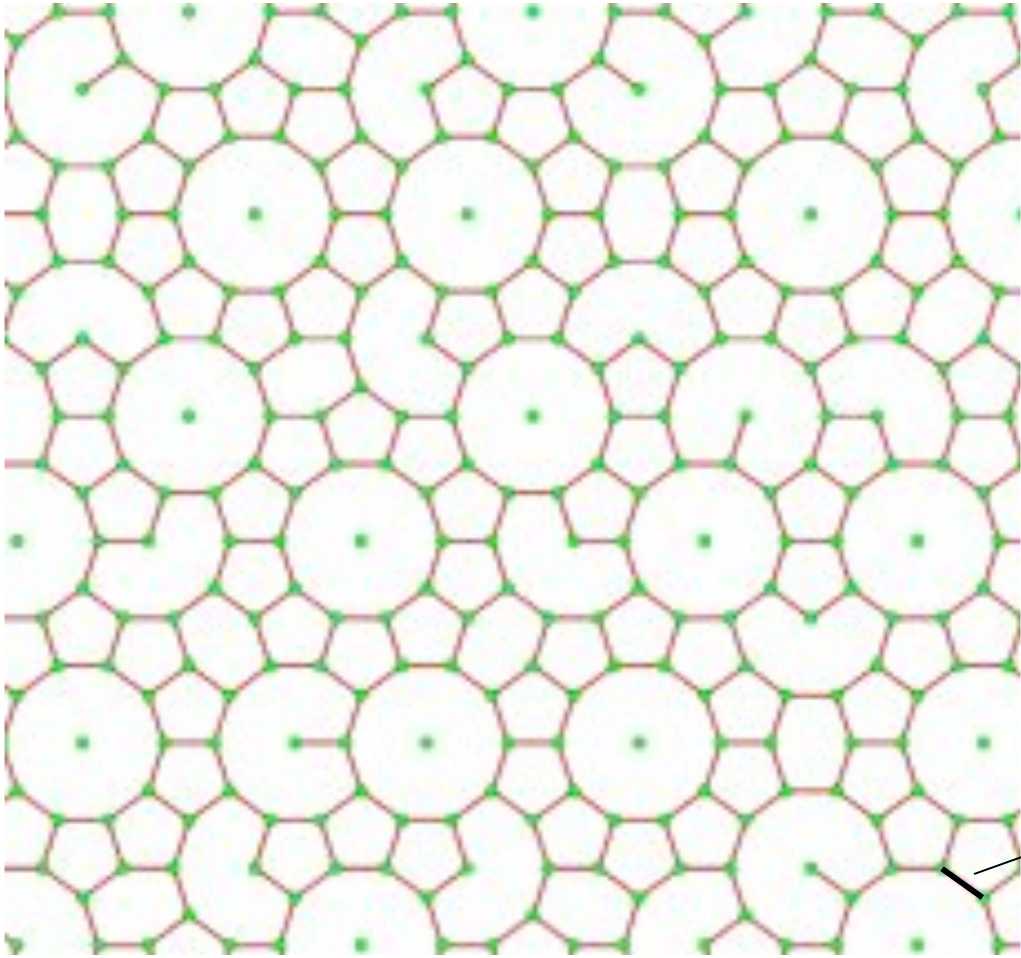
$$\Omega^{\mathrm{i}}_1 = \Omega^{\mathrm{i}}_4 = 2\tau \sin(\pi/5) a^2$$

$$\Omega^{\mathrm{i}}_2 = \Omega^{\mathrm{i}}_3 = \tau^2 \Omega^{\mathrm{i}}_1$$

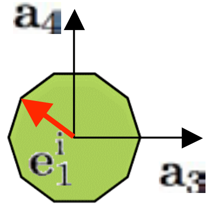
Point density: $\rho_{\mathrm{pd}} = \rho_0 \sum_\nu \Omega^{\mathrm{i}}_\nu / \Omega^{\mathrm{i}}_0 = \tau^2 \sin(\pi/5)/a^2$

Scaling of a tiling

Scale =1



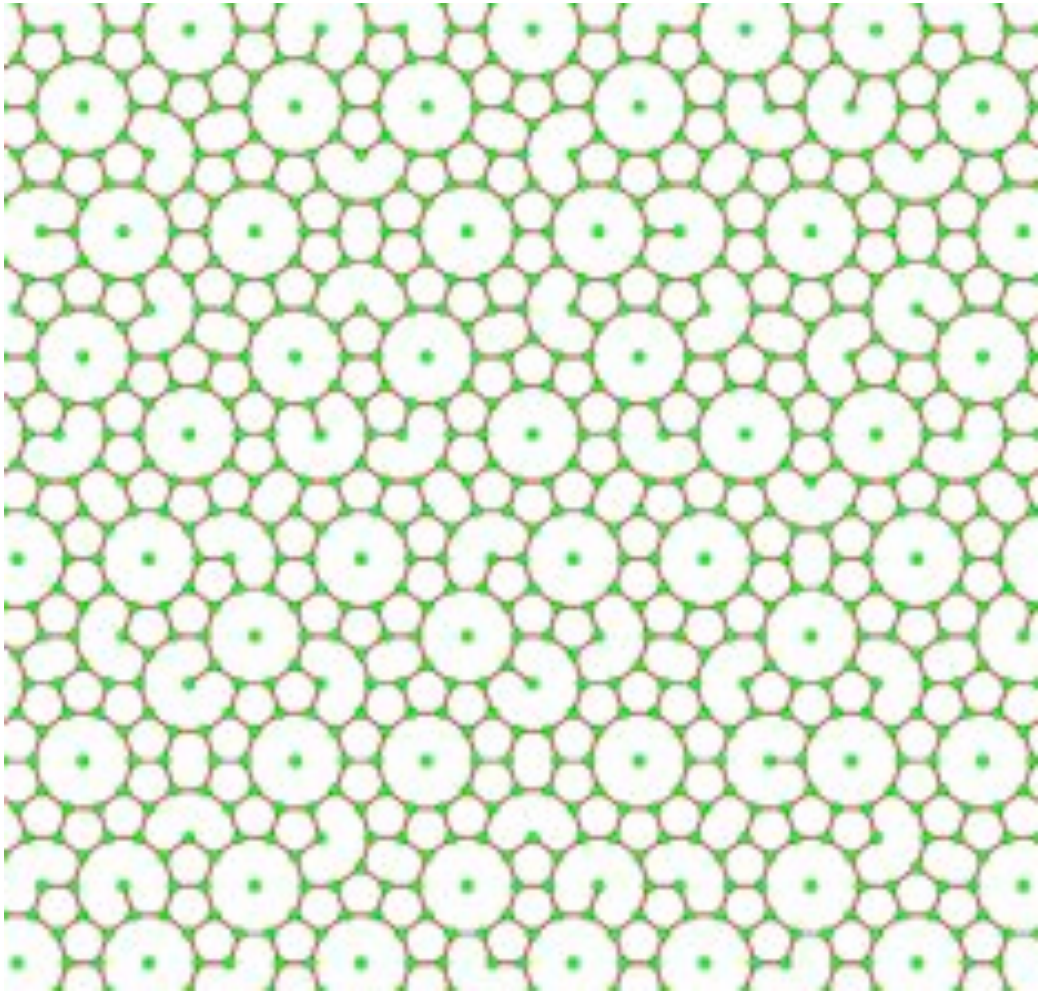
半径e_1の正10角形



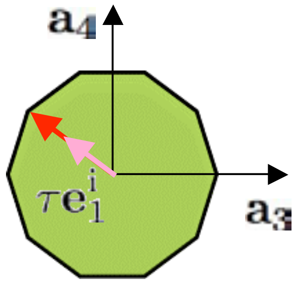
Position
: (0,0,0,0)

$\frac{2a}{\sqrt{5}}$

Scale $=\tau^{-1}$

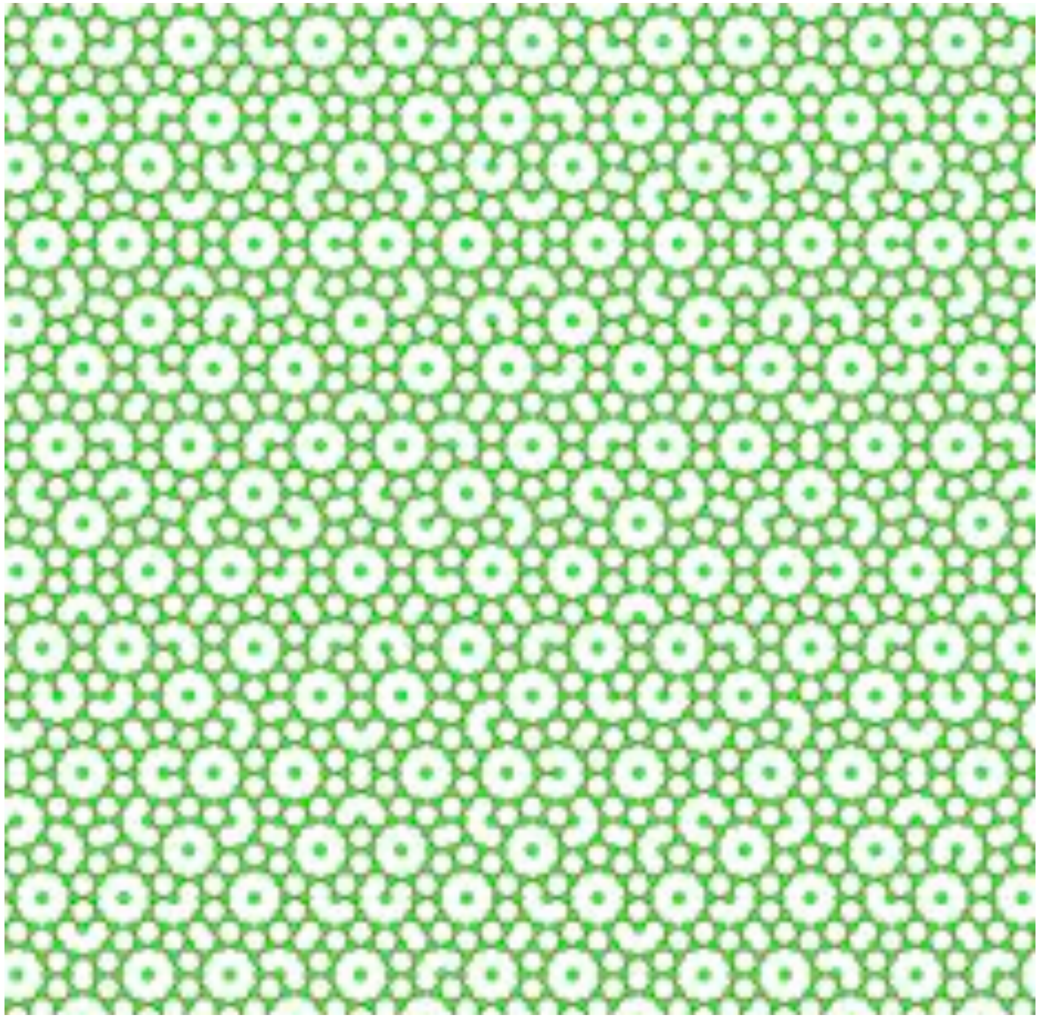


半径τ e_1の
正10角形

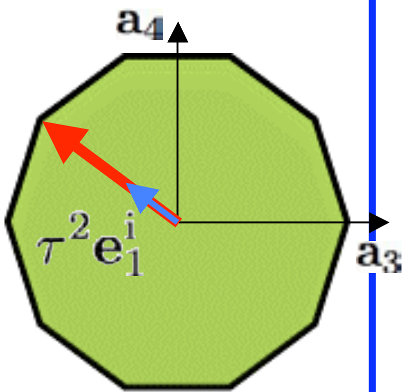


Position
:(0,0,0,0)

Scale =τ^{-2}



半径τ^2 e_1の
正10角形



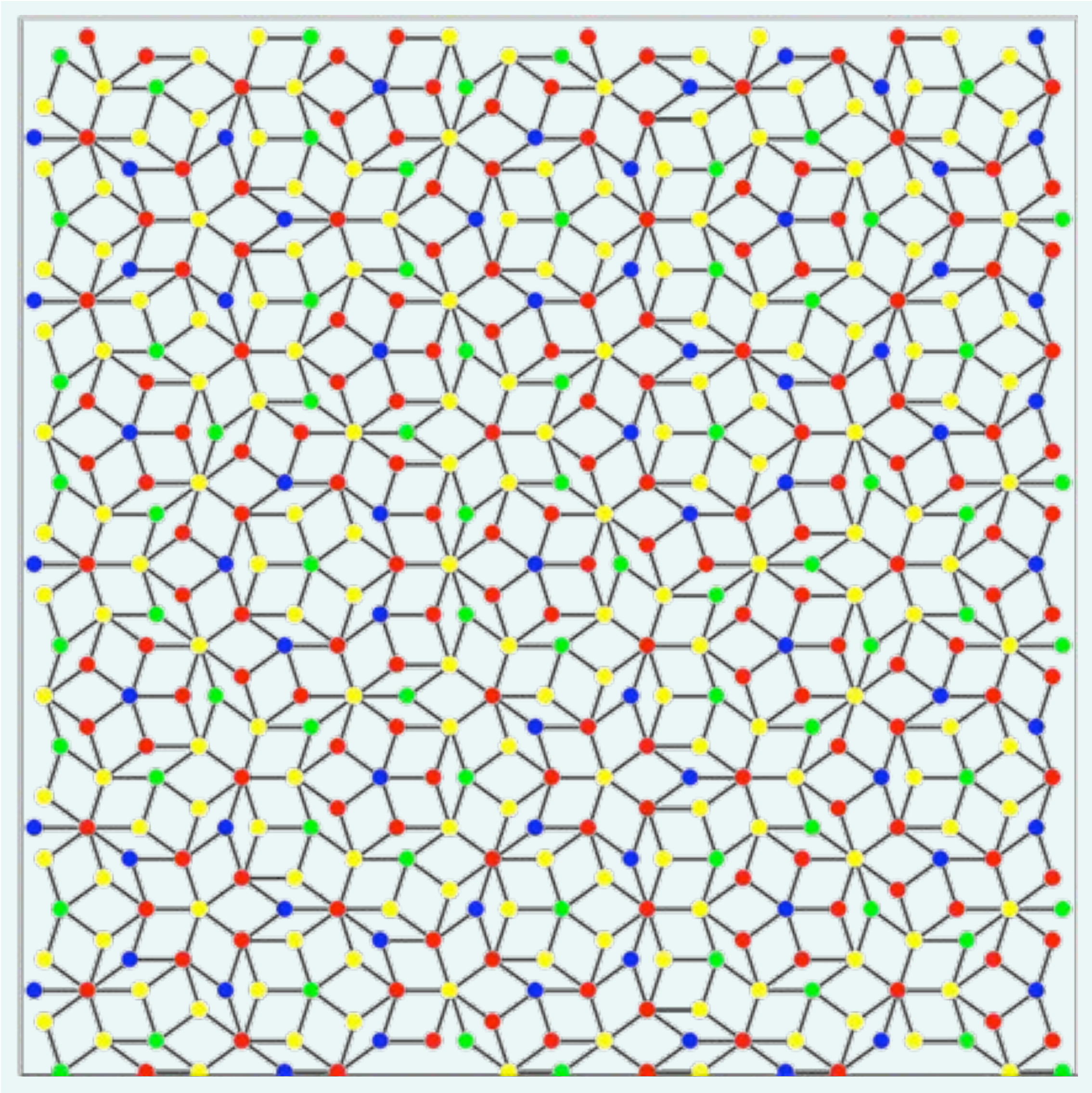
Position
:(0,0,0,0)

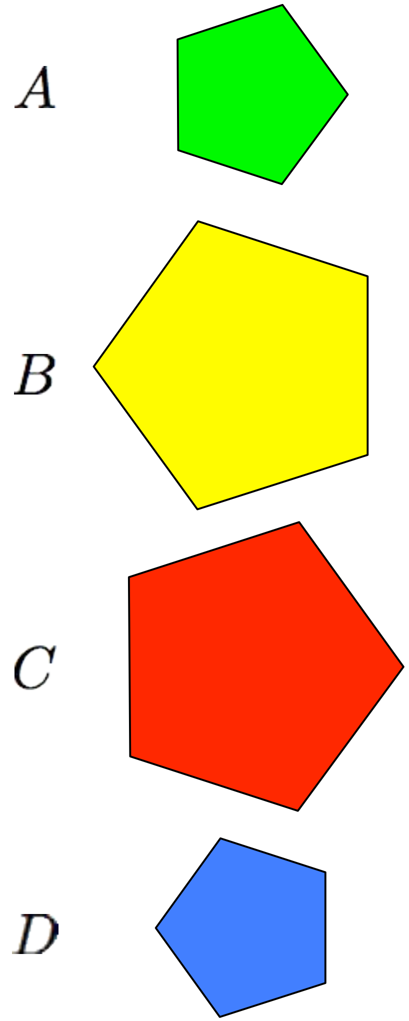
Simple models of d-QC’s

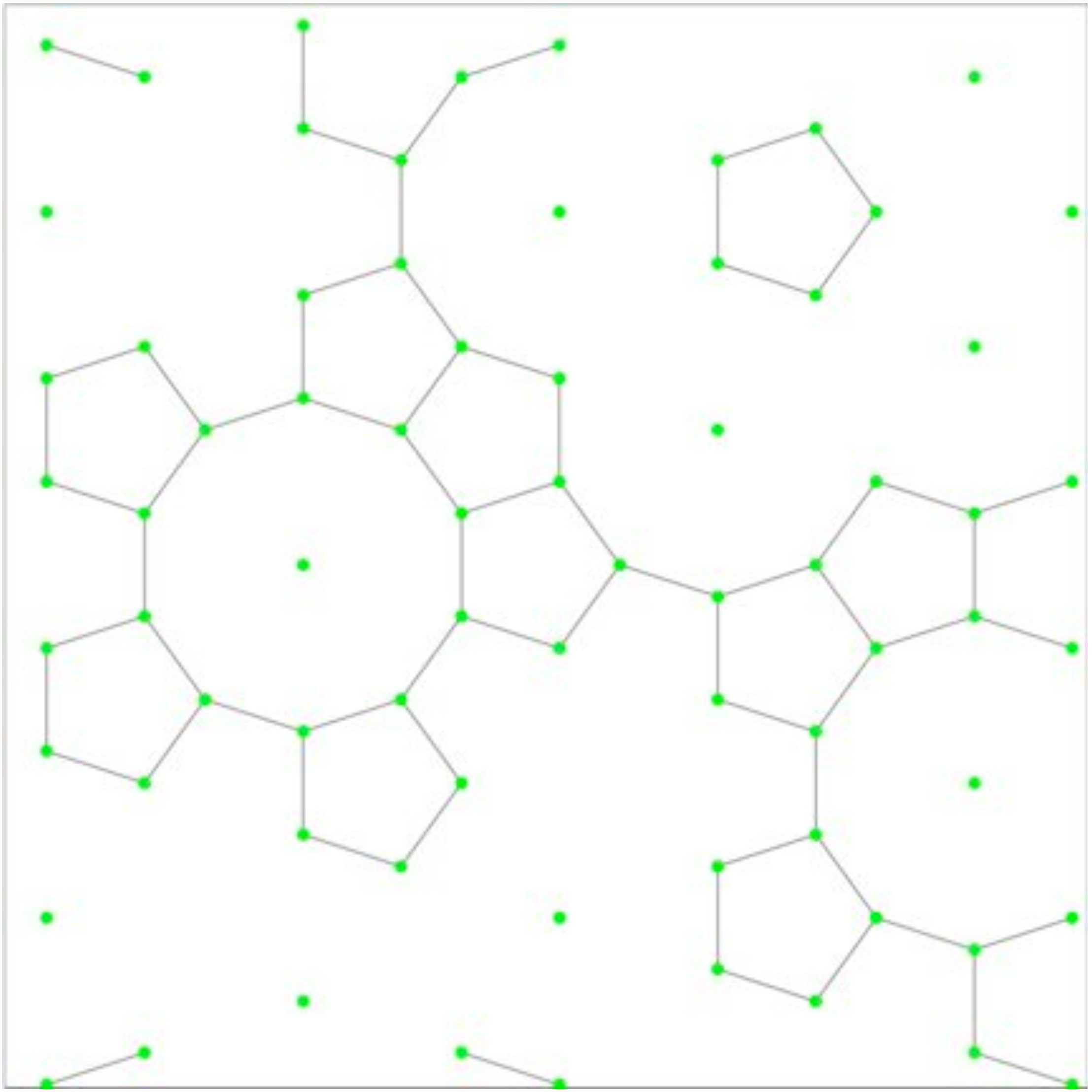
Feature of simple models

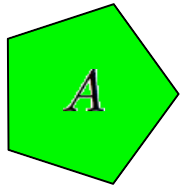
Simple models

- based on the Penrose tiling.
- explain diffraction intensity qualitatively.
- consider no atom shifts from ideal positions.
- can’t explain density.

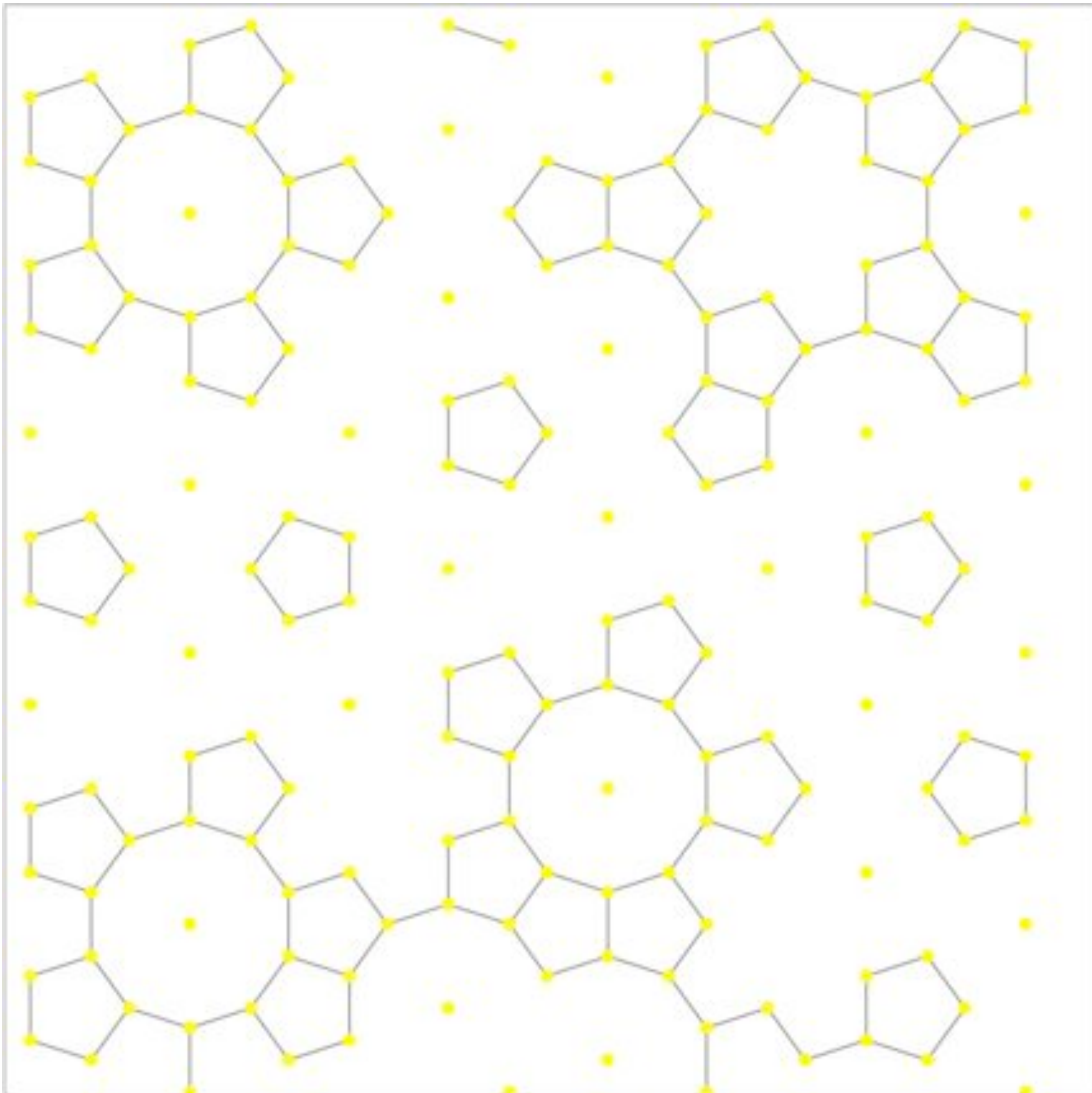


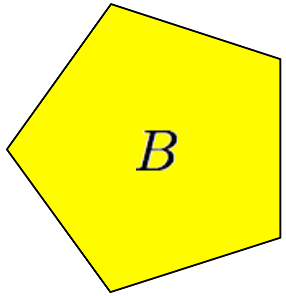

A
B
C
D



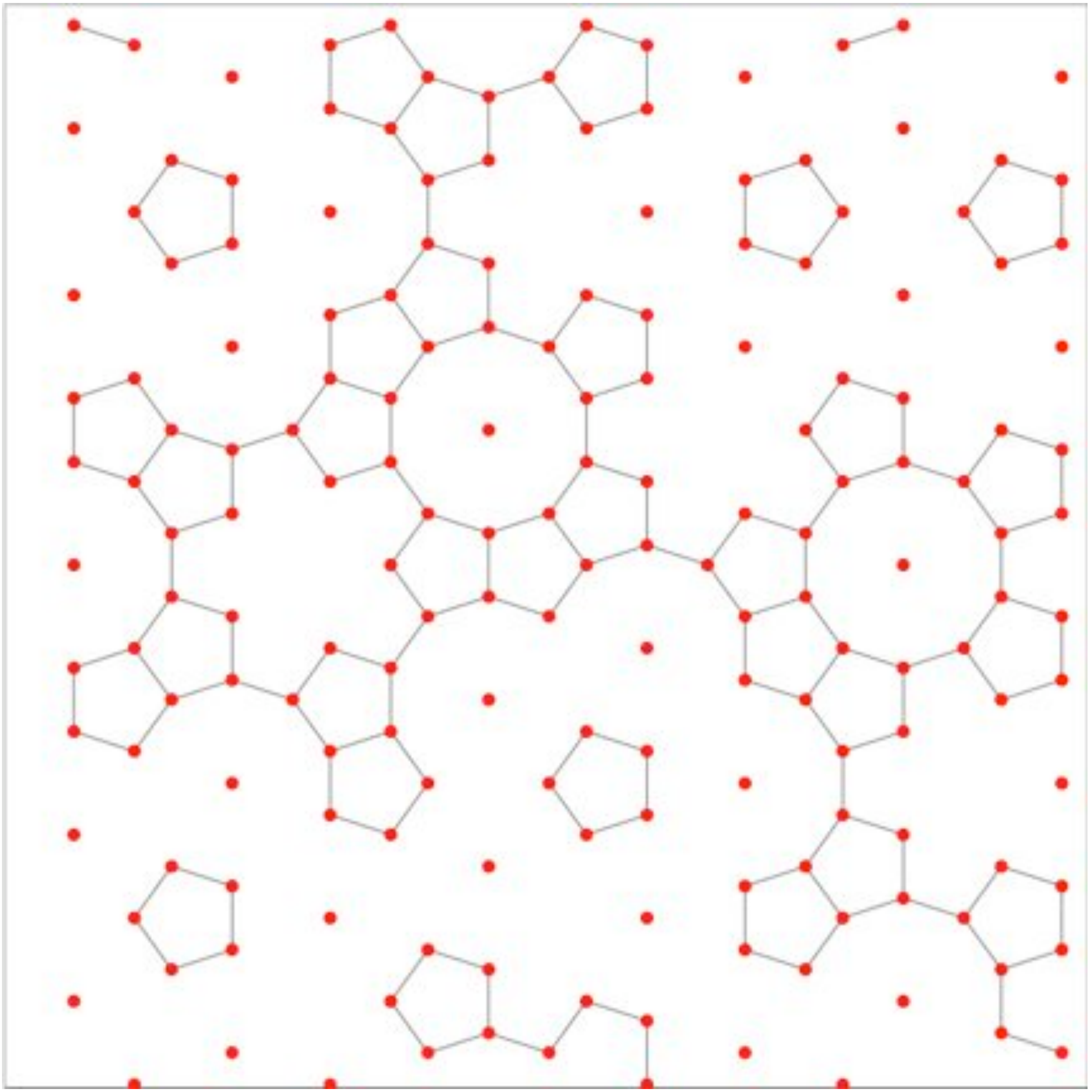


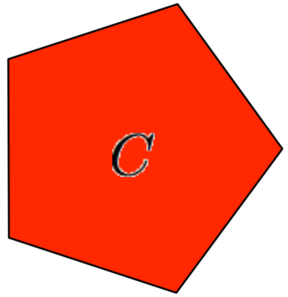
$\left(\frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}\right)$



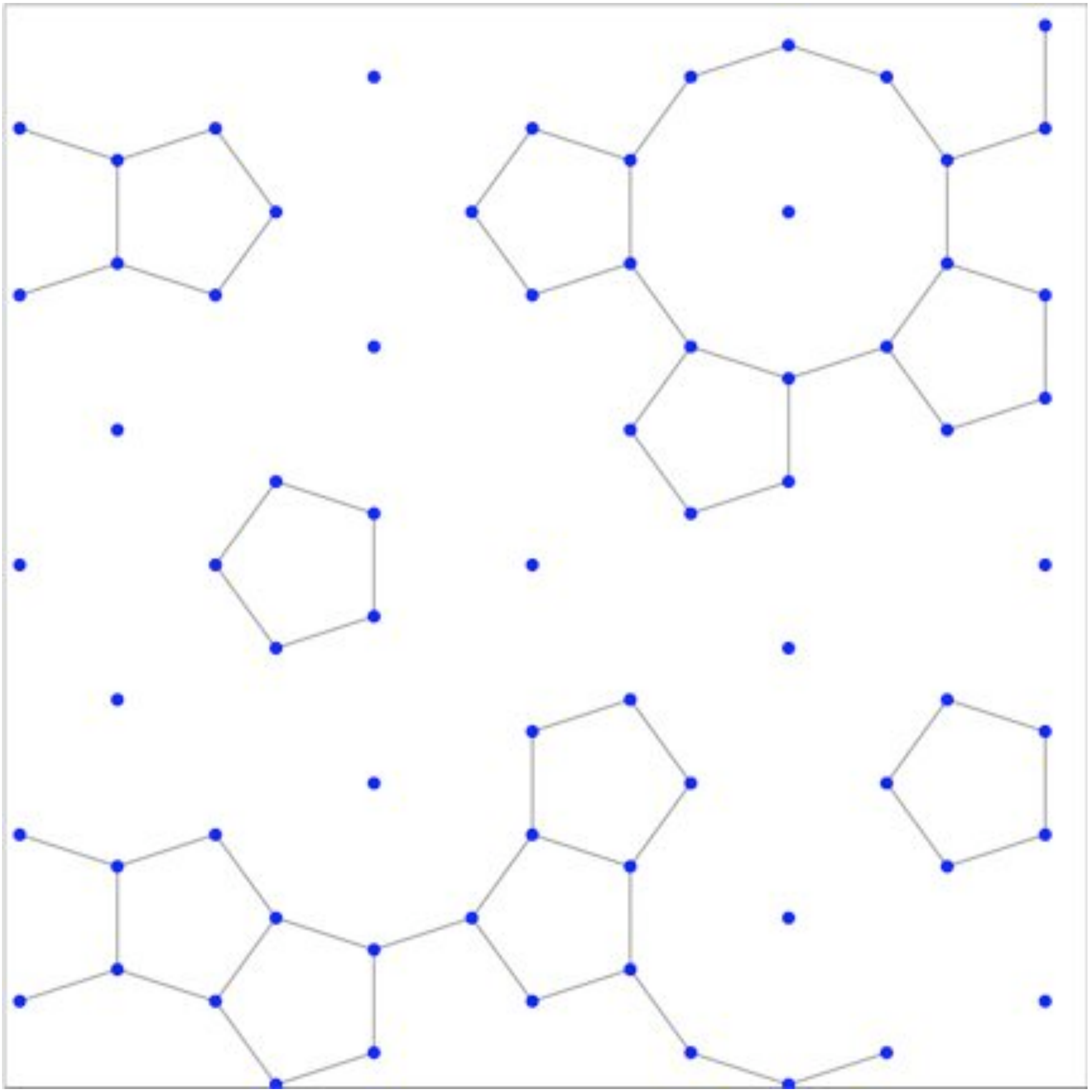


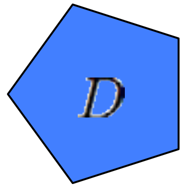
$$\left(\frac{2}{5}, \frac{2}{5}, \frac{2}{5}, \frac{2}{5}\right)$$





$$\left(\frac{3}{5}, \frac{3}{5}, \frac{3}{5}, \frac{3}{5}\right)$$





$$\left(\frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}\right)$$

Modified Al-Mn model

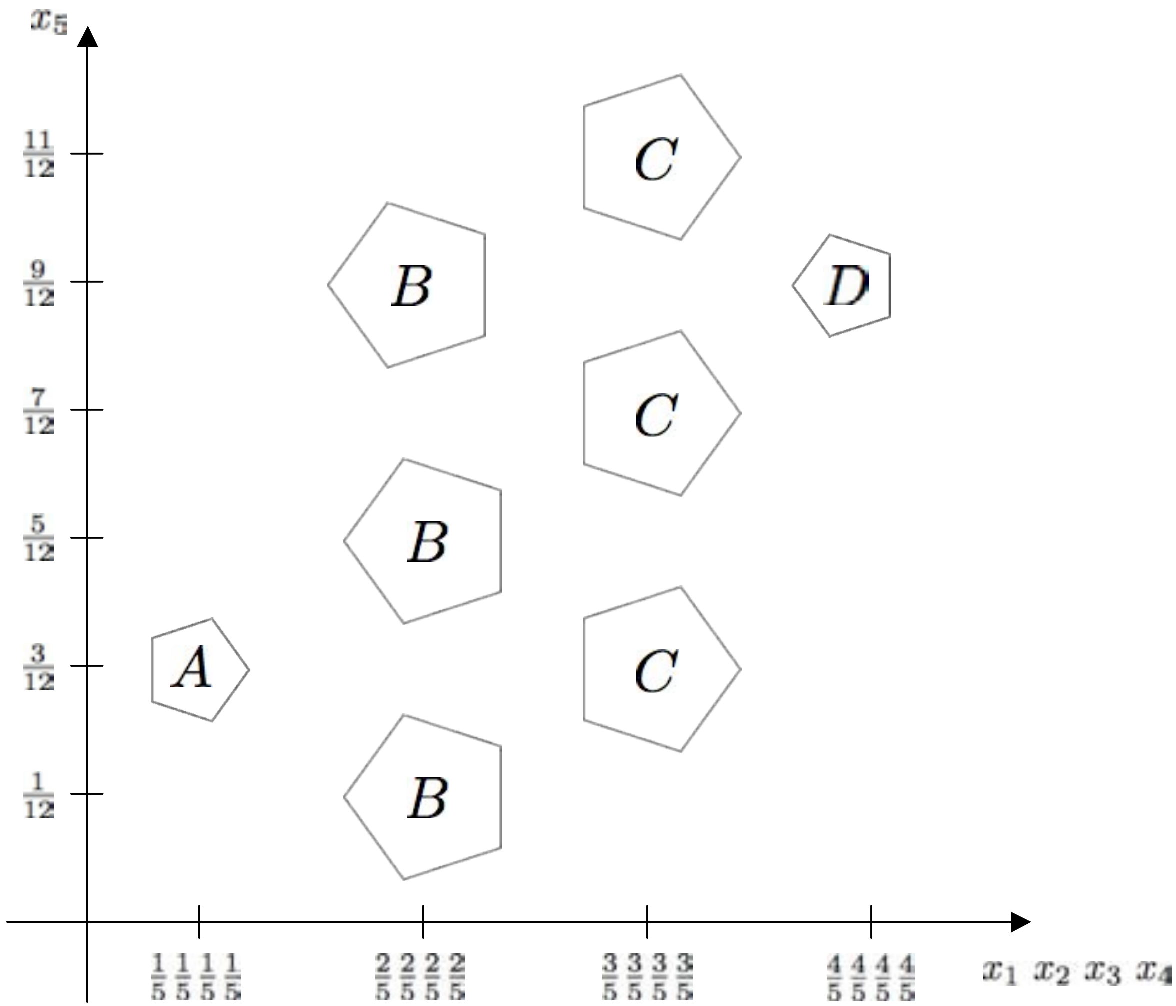
A.Yamamoto & K.N. Ishihara, Acta Cryst. (1988). **A44**, 707-714.

Space group

$P10_5/mmc$

Al-Mn: 6 layers

C
$(B+D)$
C
B
$(A+C)$
B



Modified Al-Fe model

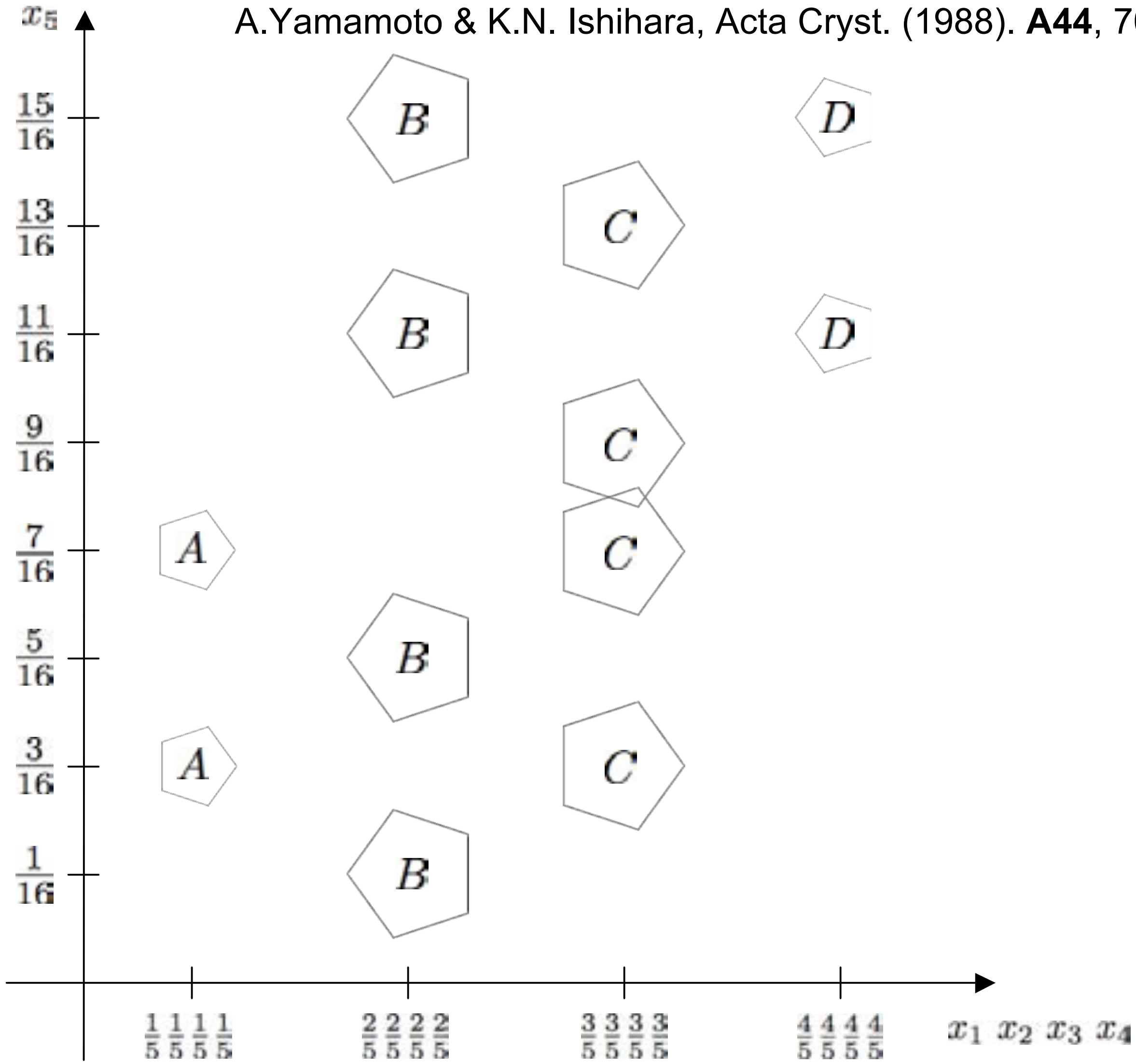
A.Yamamoto & K.N. Ishihara, Acta Cryst. (1988). **A44**, 707-714.

Space group

$P10_5mc$

Al-Fe: 8 layers

$(B+D)$
C
$(B+D)$
C
$(A+C)$
B
$(A+C)$
B



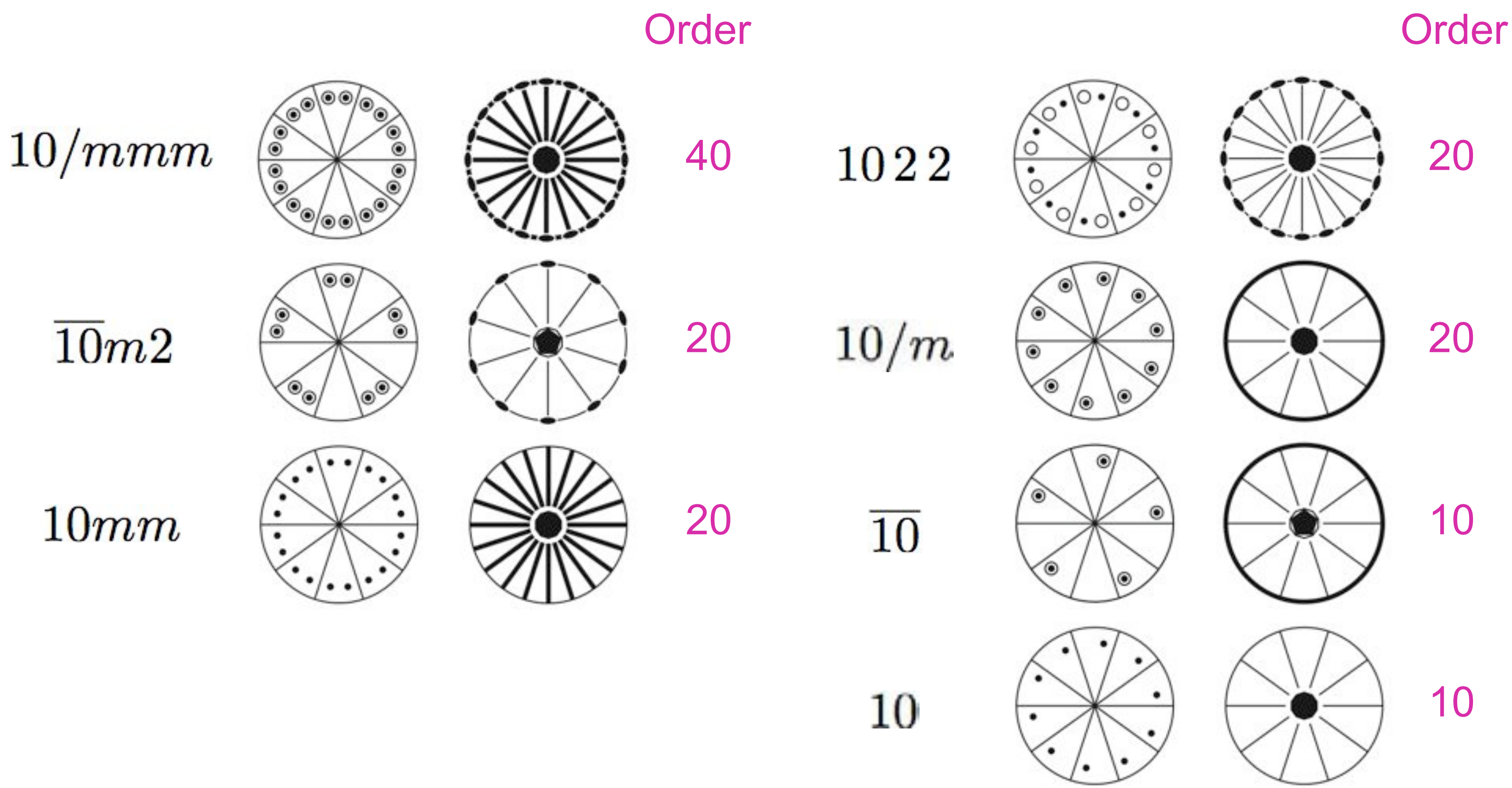
Symmetry & Space group of d-QC's in a little more details

Symmetry of d-QC's

- Symmetry reflected in diffraction patterns is that of 5D crystals.
- If a 5D crystal has a (hyper-) glide plane or (hyper-) screw axis, it cause a systematic extinction of reflections.
- Rotational symmetry ← Diffraction symmetry
- Non-primitive translation ← Reflection conditions

- In many cases, OD's are located at the special position of the space group.
- Those OD's are invariant under the site-symmetry group, which is a subgroup of the point group of the space group.
- The site symmetry restricts the shape of the OD, since the shape has to be invariant under the site-symmetry group.

Decagonal point groups



Decagonal space groups with reflection conditions

Point group	Order	Space group	Reflection condition	Point group	Order	Space group	Reflection condition
$10/mmm$	40	$P10/mmm$	no condition	$10mm$	20	$P10mm$	no condition
		$P10/mcc$	$h_5 = 2n$ for $h_1h_2h_2h_1h_5$ $h_5 = 2n$ for $h_1h_2\overline{h_2h_1}h_5$			$P10cc$	$h_5 = 2n$ for $h_1h_2h_2h_1h_5$ $h_5 = 2n$ for $h_1h_2\overline{h_2h_1}h_5$
		$P10_5/mmc$	$h_5 = 2n$ for $h_1h_2\overline{h_2h_1}h_5$			$P10_5mc$	$h_5 = 2n$ for $h_1h_2\overline{h_2h_1}h_5$
		$P10_5/mcm$	$h_5 = 2n$ for $h_1h_2h_2h_1h_5$			$P10_5cm$	$h_5 = 2n$ for $h_1h_2h_2h_1h_5$
$10/m$	20	P10/m	no condition	$\overline{10}m2$	20	$P\overline{10}m2$	no condition
		$P10_5/m$	$h_5 = 2n$ for $0000h_5$			$P\overline{10}c2$	$h_5 = 2n$ for $h_1h_2h_2h_1h_5$
1022	20	$P1022$	no condition			$P\overline{10}2m$	no condition
		$P10_j22$	$jh_5 = 10n$ for $0000h_5$			$P\overline{10}2c$	$h_5 = 2n$ for $h_1h_2\overline{h_2h_1}h_5$
				$\overline{10}$	10	$P\overline{10}$	no condition
				10	10	$P10$	no condition
						$P10_j$	$jh_5 = 10n$ for $0000h_5$

Cf. D.A.Rabson *et al.*, *Rev. Mod. Phys.* **63** (1990) 699-733.

Space group $P10_5/mmc$

Similar to $P6_3/mmc$

Point group : $10/mmm \qquad (D_{10h})$

Generators :

- tenfold screw : $\{C_{10}|\mathbf{t}(C_{10})\}$
- glide plane : $\{\sigma'|\mathbf{t}(\sigma')\}$
- inversion : $\{I|0\}$
- lattice translations : $\{E|\mathbf{d}_i\}, \qquad (i = 1, 2, 3, 4, 5)$

Non-primitive translation vector : $\mathbf{t}(C_{10}) = \mathbf{t}(\sigma') = \dfrac{\mathbf{d}_5}{2} = \dfrac{c\,\mathbf{a}_5}{2}$

Matrix representation of the generators of 5D space group $P10_5/mmc$

(hyper-) screw

$\{C_{10}|0000\tfrac{1}{2}\}$

$$R(C_{10}) = \begin{bmatrix} 0 & 0 & 0 & -1 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

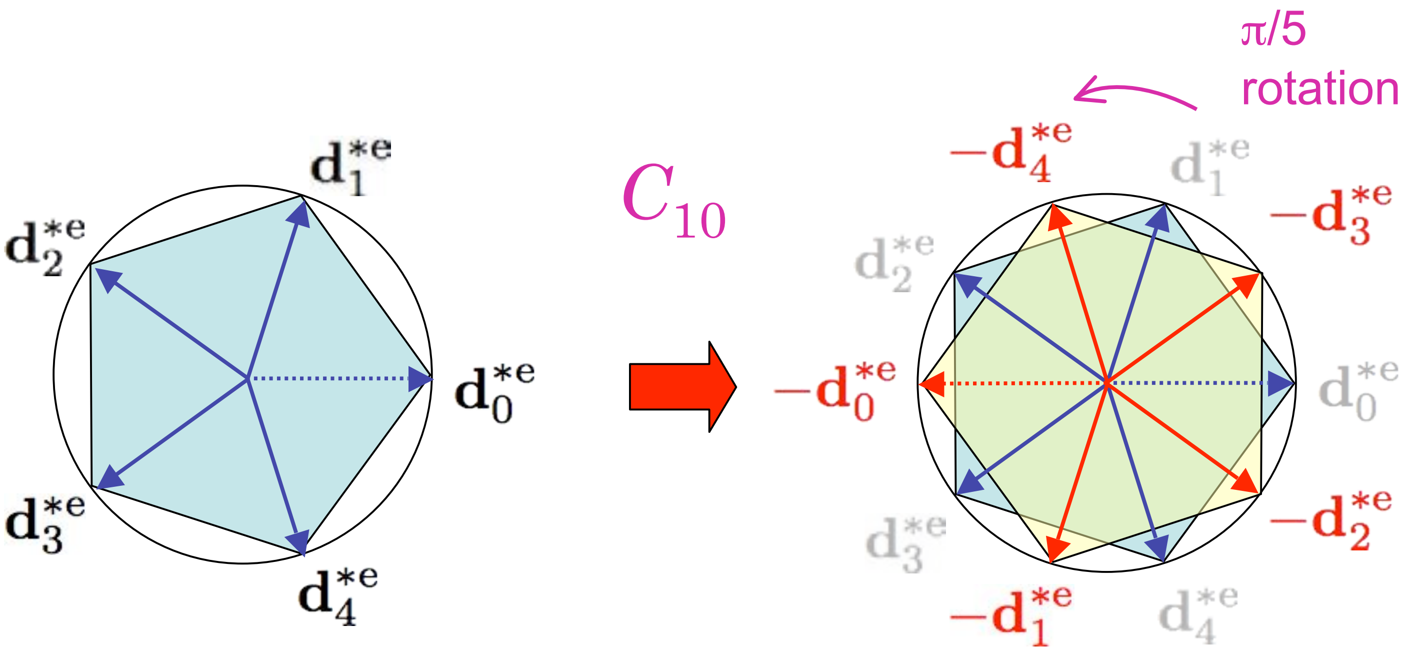
(hyper-) glide plane

$\{\sigma'|0000\tfrac{1}{2}\}$

$$R(\sigma') = \begin{bmatrix} 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$R(I) = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

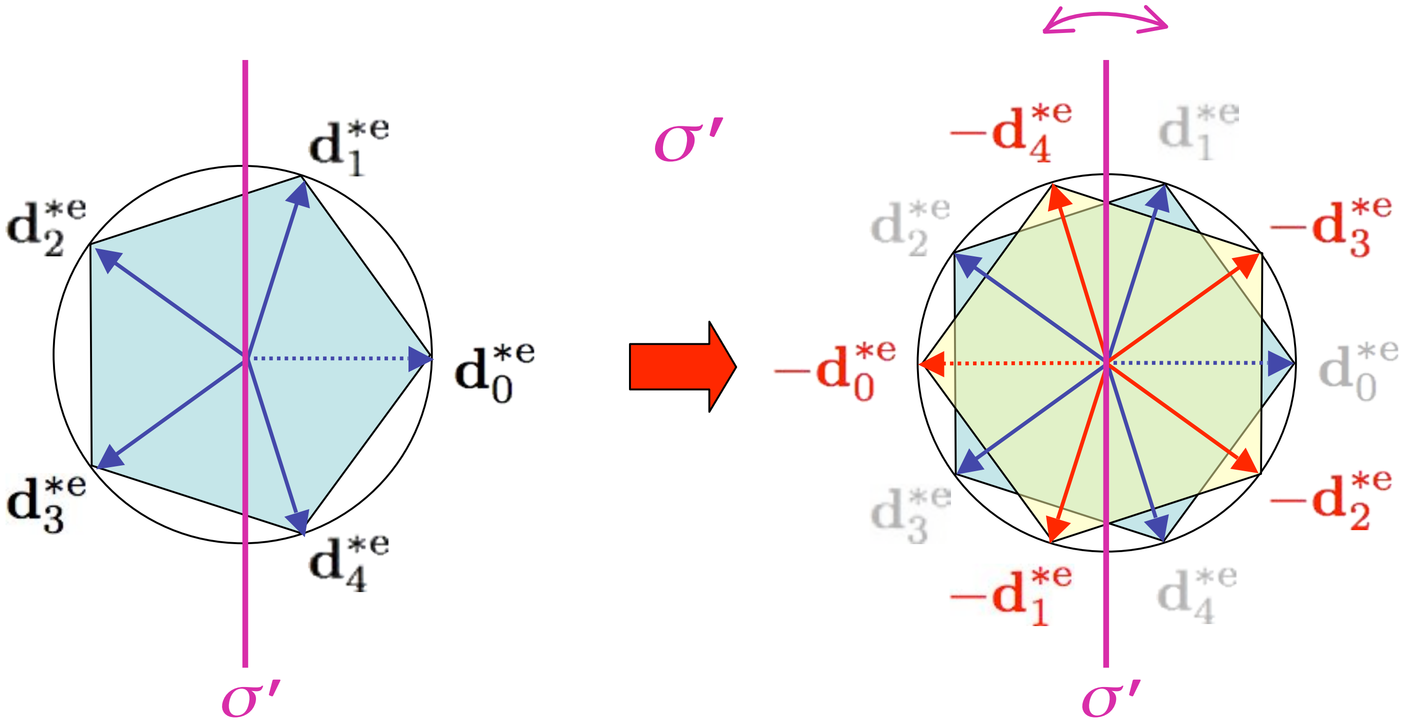
C_{10} and its action



$$\mathbf{d}_0^{*e} = -\mathbf{d}_1^{*e} - \mathbf{d}_2^{*e} - \mathbf{d}_3^{*e} - \mathbf{d}_4^{*e}$$

$$R(C_{10}) = \begin{bmatrix} 0 & 0 & 0 & -1 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

σ' and its action



$$R(\sigma') = \begin{bmatrix} 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

What to Remember

A Vector in the external or internal space is transformed into a vector in the same space by a symmetry operation.

Cluster based models of d-QC's

Cluster based model of QC's

First applied to

icosahedral quasicrystals by

A.Yamamoto and K. Hiraga, 'Structure of an icosahedral Al-Mn quasicrystal', *Physical Review* B, **37** (1988) 6207-6214.

→ model + structure refinement

decagonal quasicrystals by

S. E. Burkov, 'Structure model of the Al-Cu-Co decagonal quasicrystal', *Phys. Rev. Lett.* **67** (1991) 614-617.

→ model, no refinement

Feature of the Burkov model

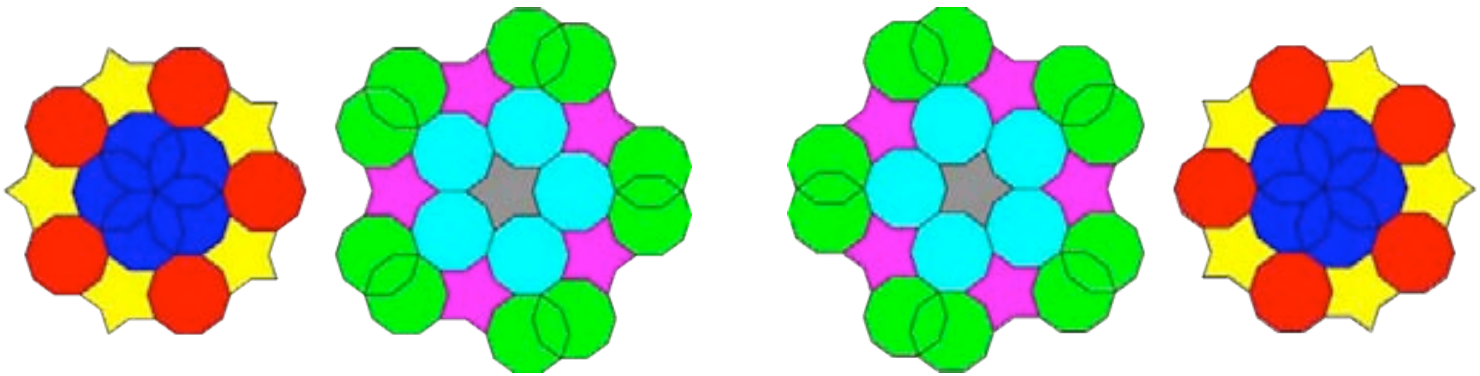
- Space group $P10_5/mmc$
- Two layered structure ~ 0.4 nm period
- Two types of atom clusters:

decagon and pentagon

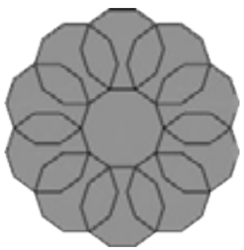
→ 2 nm 10-fold atomic cluster

→ 1.2 nm cluster linkage

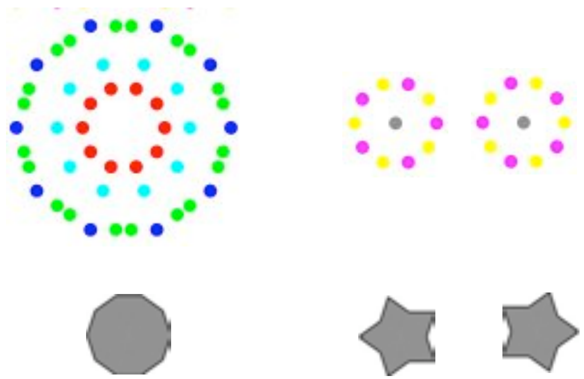
Structure model of d-Al-Cu-Co by Burkov

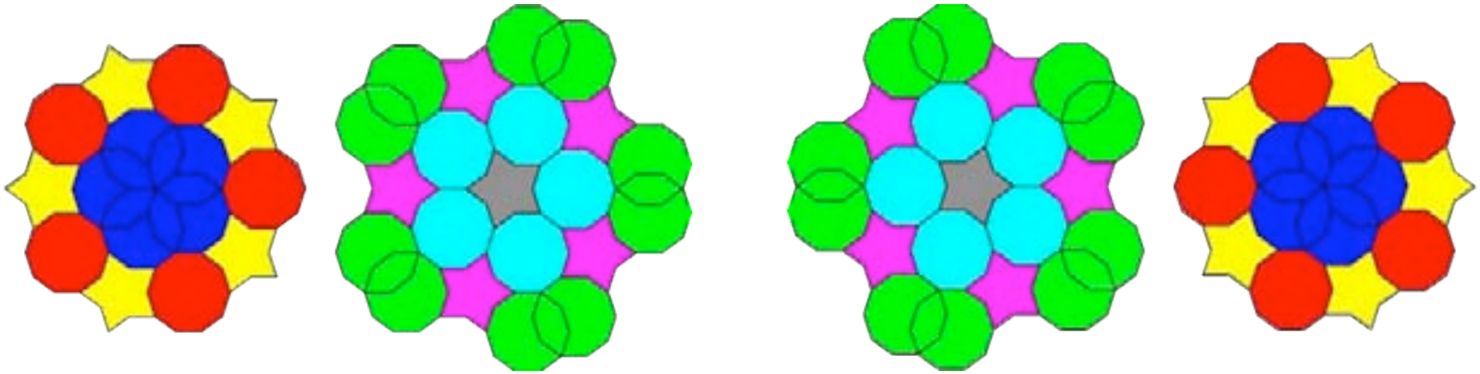


$(\frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{4})$ $(\frac{2}{5}, \frac{2}{5}, \frac{2}{5}, \frac{2}{5}, \frac{1}{4})$ $(\frac{3}{5}, \frac{3}{5}, \frac{3}{5}, \frac{3}{5}, \frac{3}{4})$ $(\frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{3}{4})$

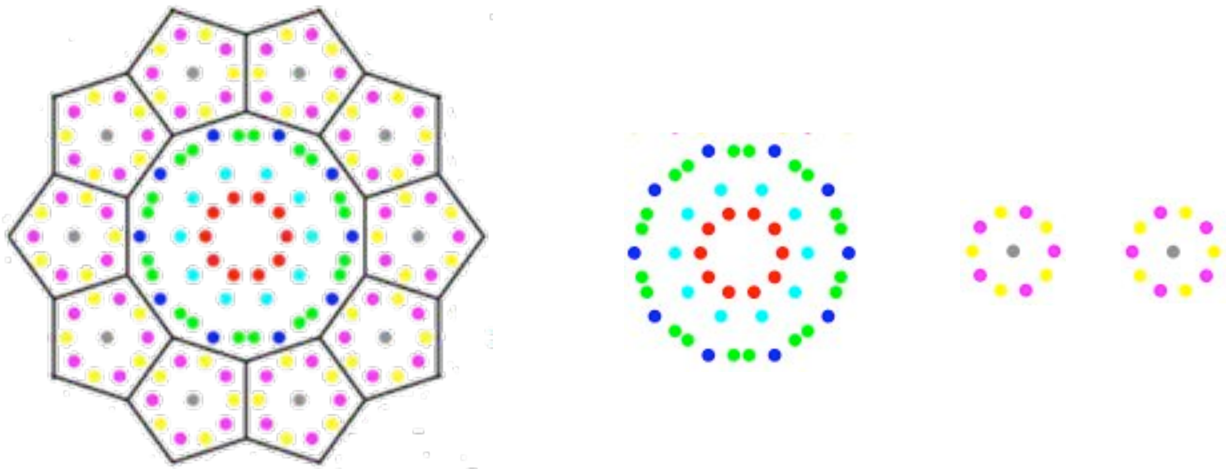


$(0, 0, 0, 0)$

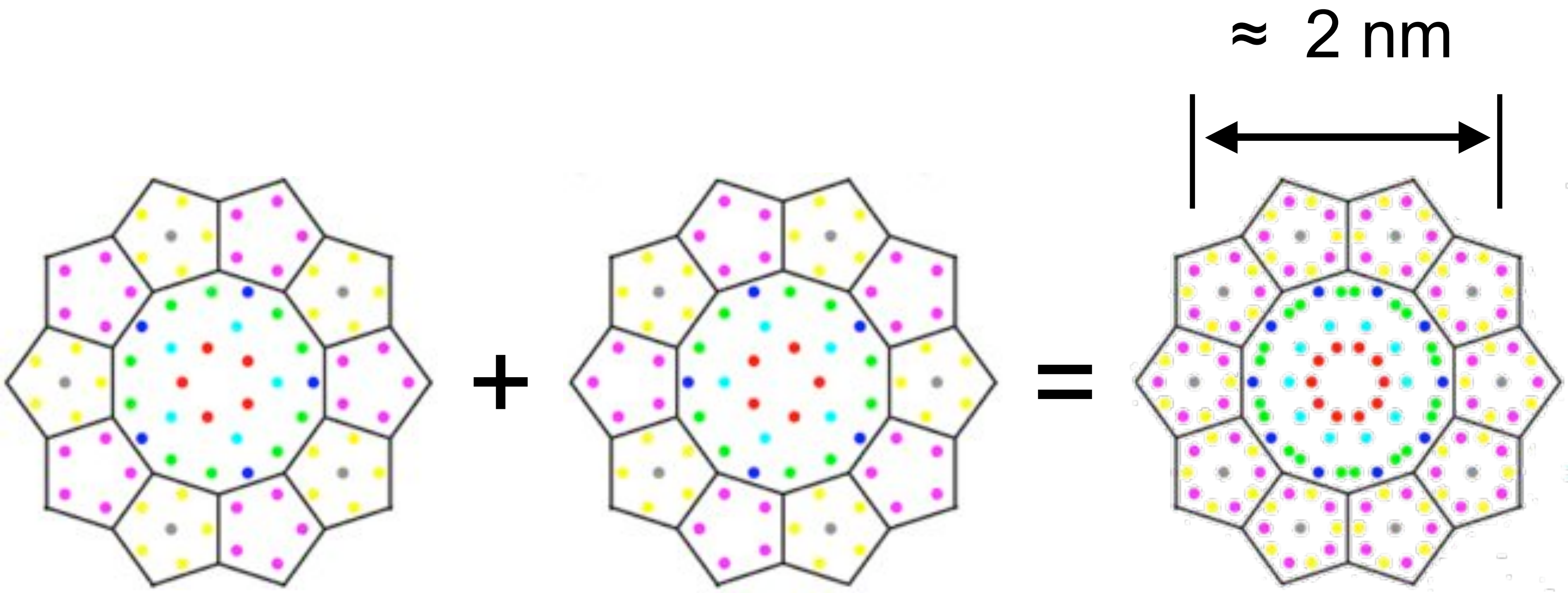




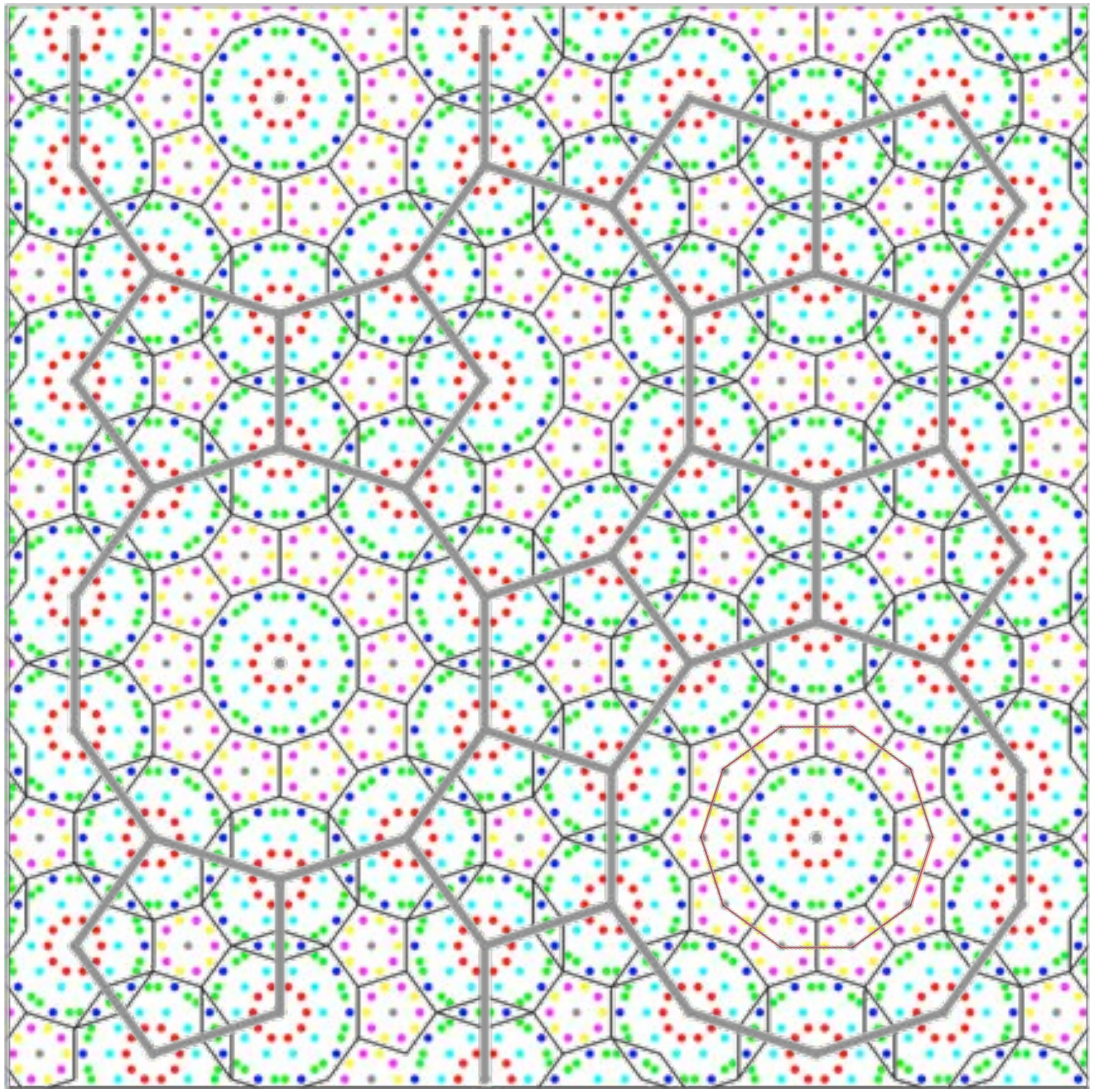
$(\frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{4})$ $(\frac{2}{5}, \frac{2}{5}, \frac{2}{5}, \frac{2}{5}, \frac{1}{4})$ $(\frac{3}{5}, \frac{3}{5}, \frac{3}{5}, \frac{3}{5}, \frac{3}{4})$ $(\frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{3}{4})$

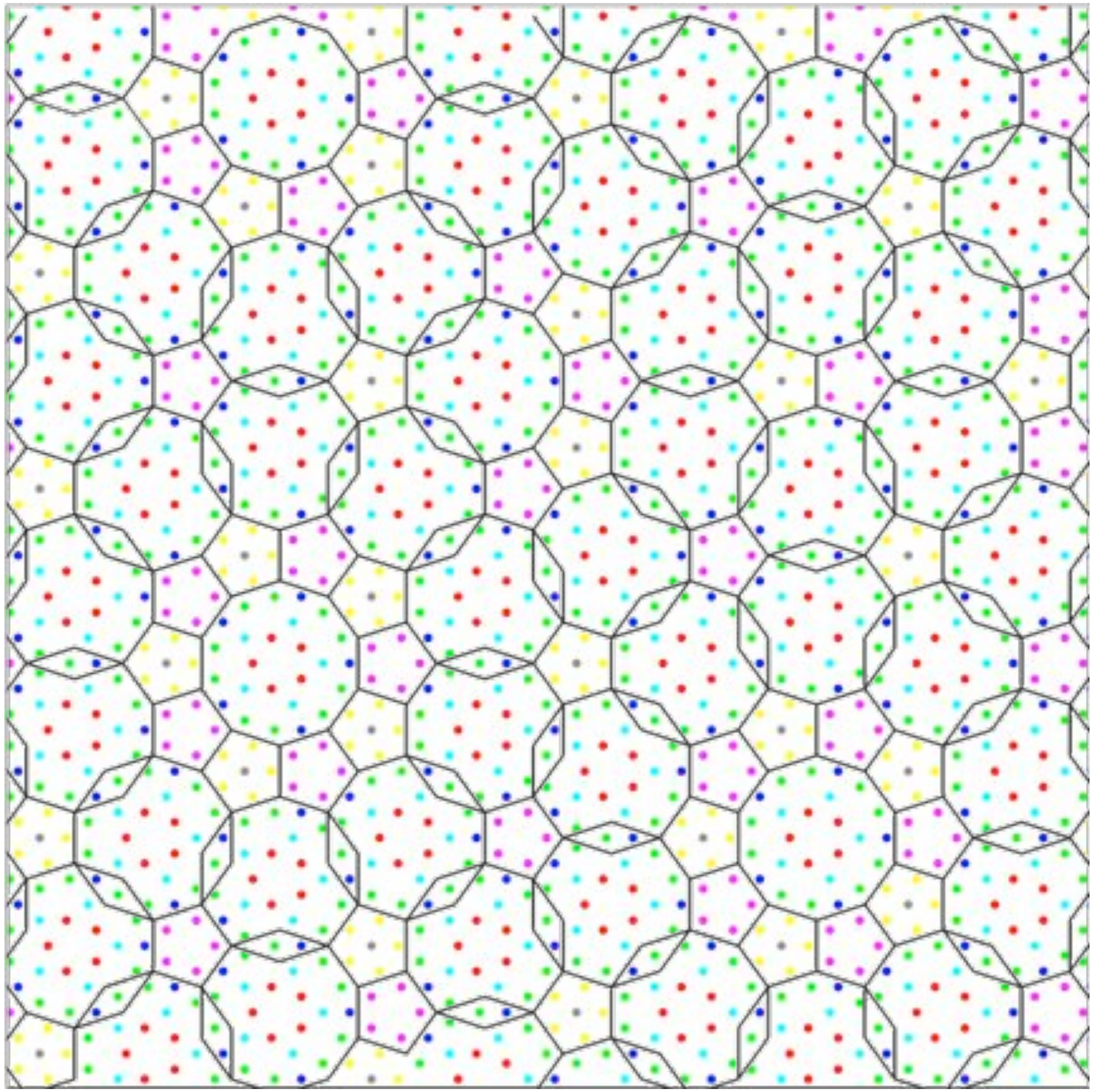


2 nm cluster in the Burkov model

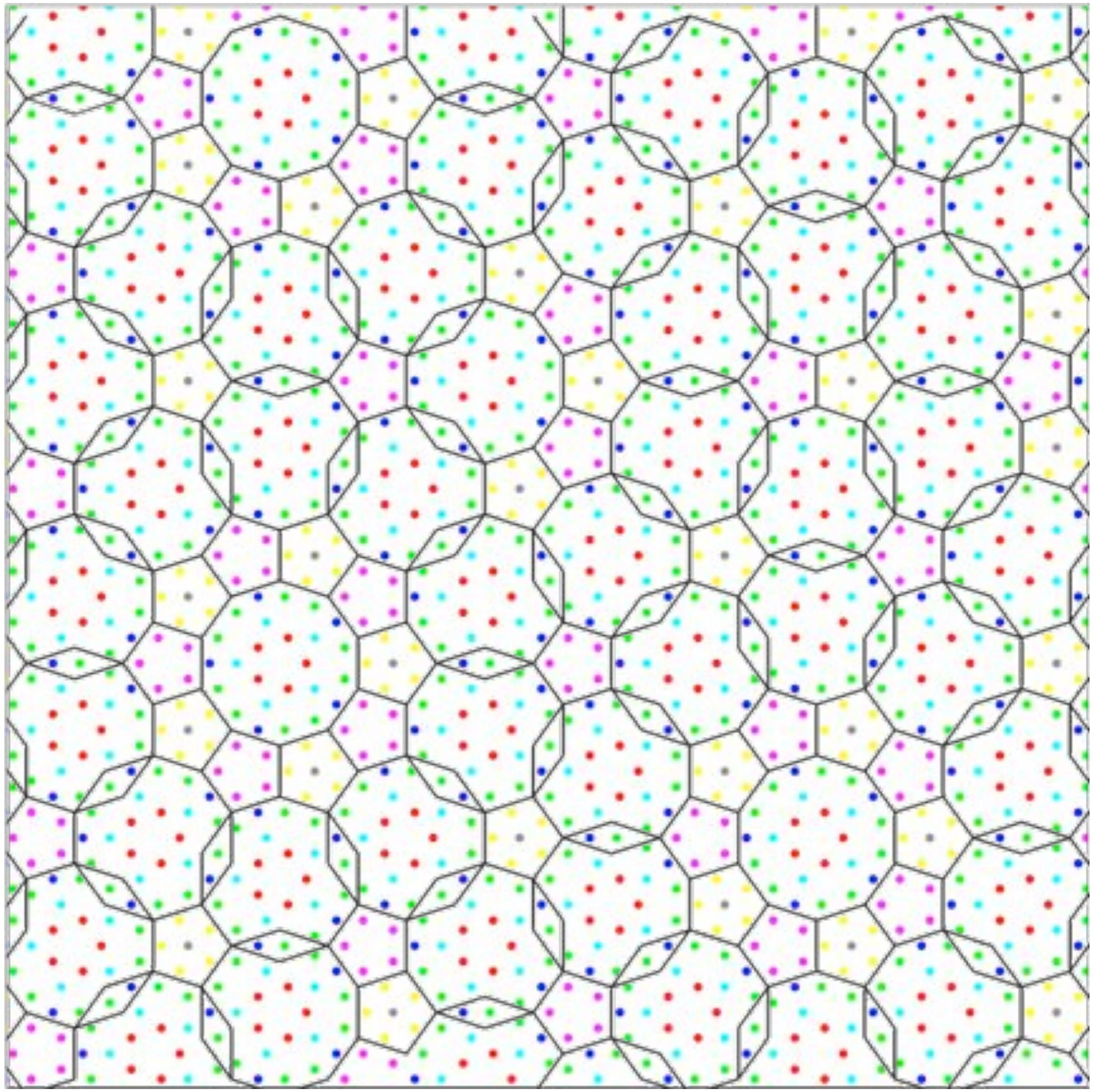


$z = \frac{1}{4}$ $z = \frac{3}{4}$ superposition





$$z = \frac{1}{4}$$



$$z = \frac{3}{4}$$

Feature of the Yamamoto 2nm model

- Space group $P10_5/mmc$
- Two layered structure ~ 0.4 nm period
- Three types of atom clusters:

decagon, pentagon, and star

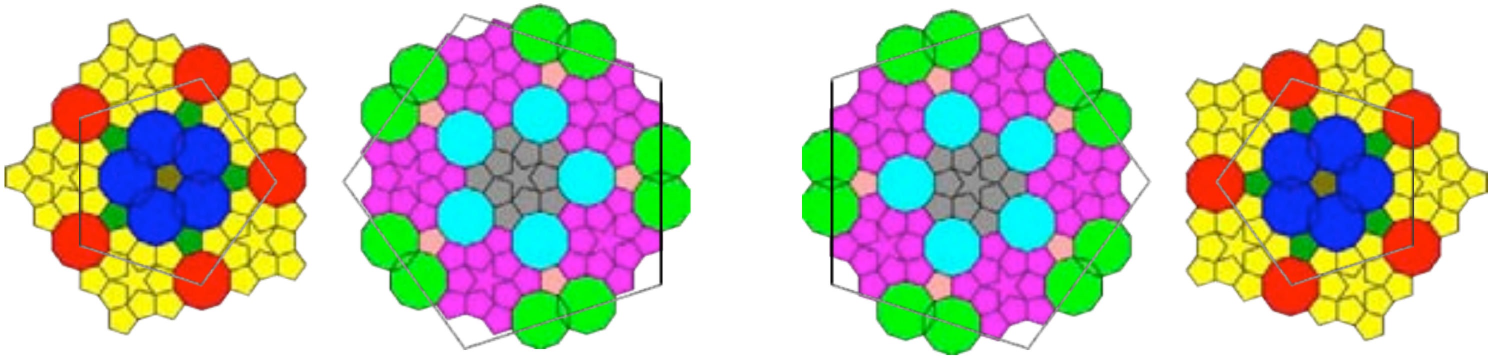
→ 2 nm 10-fold atomic cluster

→ 2 nm cluster linkage

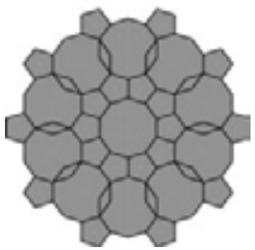
Pentagonal Penrose tiling

Yamamoto's 2 nm cluster model

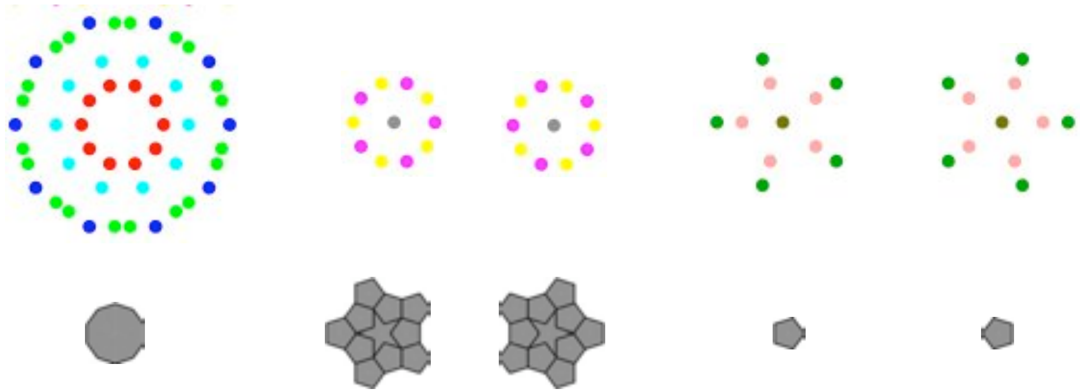
A.Yamamoto, Sci. Rep. RITU. (1996). **A42**, 207-212.

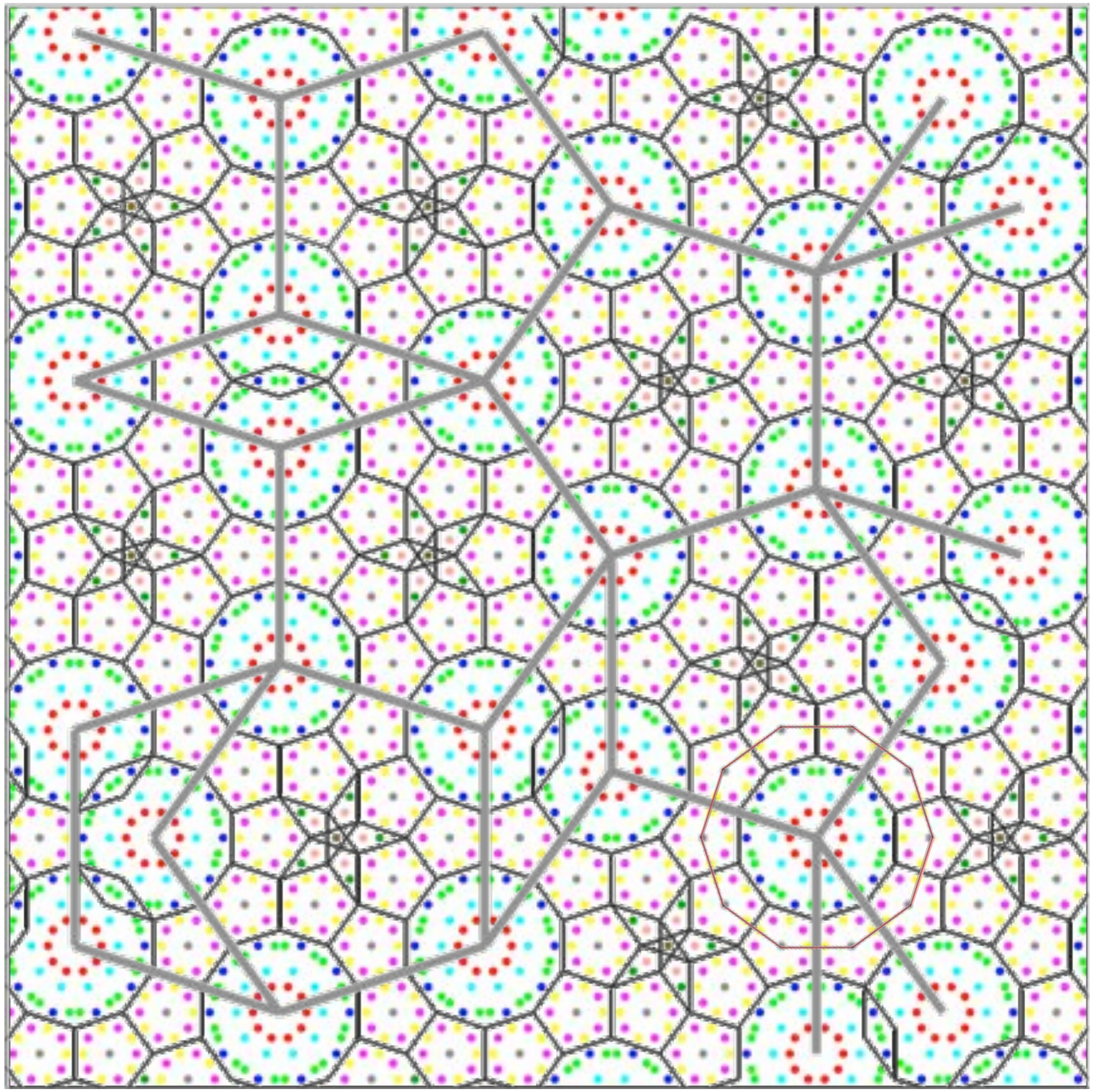


$(\frac{1}{5},\frac{1}{5},\frac{1}{5},\frac{1}{5},\frac{1}{4})$ $(\frac{2}{5},\frac{2}{5},\frac{2}{5},\frac{2}{5},\frac{1}{4})$ $(\frac{3}{5},\frac{3}{5},\frac{3}{5},\frac{3}{5},\frac{3}{4})$ $(\frac{4}{5},\frac{4}{5},\frac{4}{5},\frac{4}{5},\frac{3}{4})$

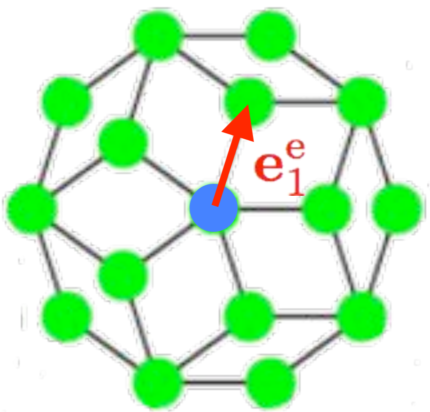


$(0,0,0,0)$





Construction of cluster based model



$$\pm\mathbf{e}_i^{\mathrm{e}} = \mp\mathbf{e}_i^{\mathrm{i}} \pm \mathbf{d}_i \mp \sum_{l=1}^{4} \mathbf{d}_l/5$$

- $\mathbf{d}_i = \mathbf{d}_i^{\mathrm{e}} + \mathbf{d}_i^{\mathrm{i}}$
- $\begin{cases} \mathbf{e}_i^{\mathrm{e}} = \mathbf{d}_i^{\mathrm{e}} - \sum_{l=1}^{4} \mathbf{d}_l^{\mathrm{e}}/5 \\ \mathbf{e}_i^{\mathrm{i}} = \mathbf{d}_i^{\mathrm{i}} - \sum_{l=1}^{4} \mathbf{d}_l^{\mathrm{i}}/5 \end{cases}$
- $\begin{aligned} \mathbf{e}_i^{\mathrm{e}} + \mathbf{e}_i^{\mathrm{i}} &= \mathbf{d}_i^{\mathrm{e}} + \mathbf{d}_i^{\mathrm{i}} - \sum_{l=1}^{4}(\mathbf{d}_l^{\mathrm{e}}/5 + \mathbf{d}_l^{\mathrm{i}}/5) \\ &= \mathbf{d}_i - \sum_{l=1}^{4}\mathbf{d}_l/5 \end{aligned}$

$$\mathbf{e}_i^{\mathrm{e}} = \frac{2a}{\sqrt{5}}[c_i\mathbf{a}_1 + s_i\mathbf{a}_2]$$

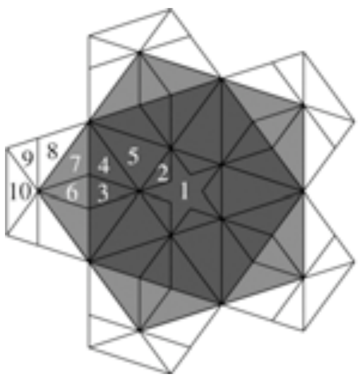
$$(i = 1, 2, 3, 4)$$

$$|\mathbf{e}_i^{\mathrm{i}}| = \frac{2a}{\sqrt{5}}$$

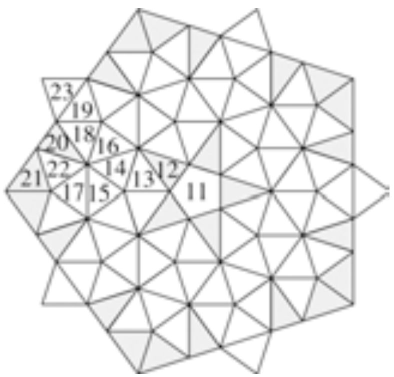
$$\begin{aligned} \mathbf{e}_1^{\mathrm{e}} &= -\mathbf{e}_1^{\mathrm{i}} + \mathbf{d}_1 - \sum_{l=1}^{4}\mathbf{d}_l/5 \\ &= -\mathbf{e}_1^{\mathrm{i}} + \tfrac{4}{5}\mathbf{d}_1 - \tfrac{1}{5}\mathbf{d}_2 - \tfrac{1}{5}\mathbf{d}_3 - \tfrac{1}{5}\mathbf{d}_4 \\ &\equiv -\mathbf{e}_1^{\mathrm{i}} - \sum_{l=1}^{4}\mathbf{d}_l/5 \end{aligned}$$

Refined structure of d-$Al_{72}Ni_{20}Co_8$ QC

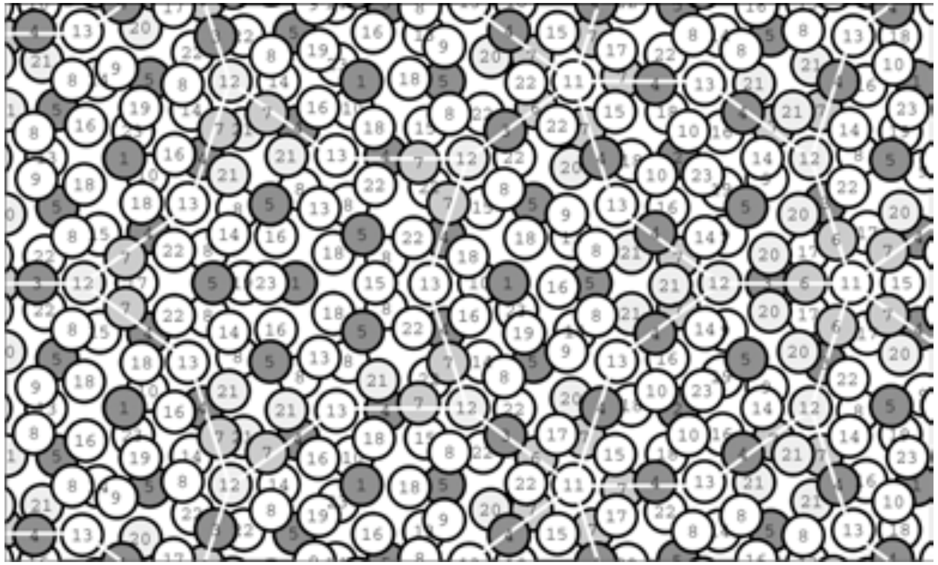
Space group $P10_5/mmc$



$(\frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{4})$



$(\frac{2}{5}, \frac{2}{5}, \frac{2}{5}, \frac{2}{5}, \frac{1}{4})$



H.Takakura, A.Yamamoto, A.P.Tsai, Acta Cryst. (2001). **A57**, 576-585.

Structure-factor formula for QC's

Structure factor formula

$$F(\mathbf{h}) = \sum_{\mu} \sum_{\{R|\mathbf{t}\}^{\mu}} f^{\mu}(\mathbf{h}^{\mathrm{e}}) p^{\mu} \exp\{-B^{\mu}(\mathrm{h}^{\mathrm{e}})^2/4\}$$
$$\times \exp\{2\pi i\, \mathbf{h} \cdot (R\, \mathbf{r}^{\mu} + \mathbf{t})\} F_0^{\mu}(R^{-1}\mathbf{h})$$

μ : Independent occupation domain

$\{R|\mathbf{t}\}^{\mu}$: Symmetry operators of space group which generate equivalent occupation domains in a unit cell from the independent occupation domain μ

Provided that the occupation domain consists of ν independent triangles (or tetrahedra), it is given by

$$F_0^{\mu}(\mathbf{h}) = \sum_{i=1}^{\nu} \sum_{R'} F_{0i}^{\mu}(R'^{-1}\mathbf{h})$$

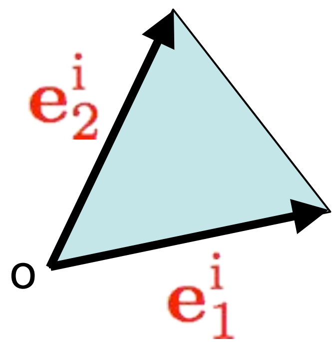
R' : Rotational part of site-symmetry operator

Fourier integral of a triangle

$$F_{0i}^{\mu}(\mathbf{h}) = \frac{V\left[q_1\{\exp(iq_2)-1\} - q_2\{\exp(iq_1)-1\}\right]}{q_1 q_2 (q_1 - q_2)}$$

$$V = |\mathbf{e}_1^{\mathrm{i}} \times \mathbf{e}_2^{\mathrm{i}}|,$$

$$q_j = 2\pi \mathbf{e}_j^{\mathrm{i}} \cdot \mathbf{h}^{\mathrm{i}} \quad (j = 1, 2).$$



Asymmetric part

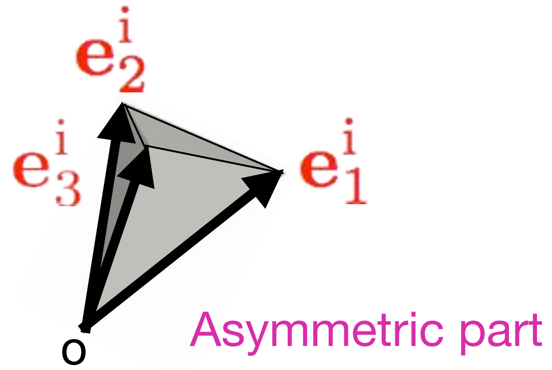
Fourier integral of a tetrahedron

$$F_{0i}^{\mu}(\mathbf{h}) = -iV \frac{q_2 q_3 q_4 \exp(iq_1) + q_3 q_1 q_5 \exp(iq_2) + q_1 q_2 q_6 \exp(iq_3) + q_4 q_5 q_6}{q_1 q_2 q_3 q_4 q_5 q_6}$$

$$q_j = 2\pi \mathbf{h}^{\mathrm{i}} \cdot \mathbf{e}_j^{\mathrm{i}} \quad (j = 1, 2, 3),$$

$$q_4 = q_2 - q_3, \quad q_5 = q_3 - q_1, \quad q_6 = q_1 - q_2,$$

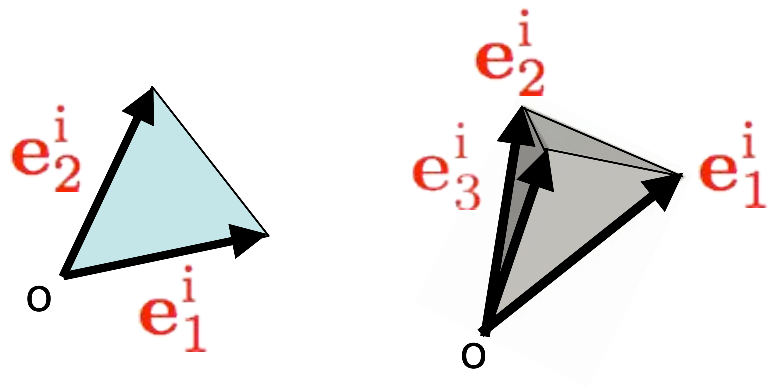
$$V = \mathbf{e}_1^{\mathrm{i}} \cdot [\mathbf{e}_2^{\mathrm{i}} \times \mathbf{e}_3^{\mathrm{i}}]$$



Structural parameters for QC's

- Position
- ADP
- Occupancy
- Ratio of elements

for μth occupation domain



Asymmetric parts

It is assumed that the shape of the OD's is known.
One of the difficult problems of the structure determination is to determine the size and shape of OD's.