Point substitution processes for generating icosahedral tilings

Nobuhisa Fujita

IMRAM, Tohoku University,
Sendai 980-8577, Japan

Outline

Part I.

1. Basic icosahedral tilings
2. Point substitution processes

Part II.

3. Tilings constructed with PIRs
4. Canonical cell tilings
5. Toward icosahedral CCTs

Outline

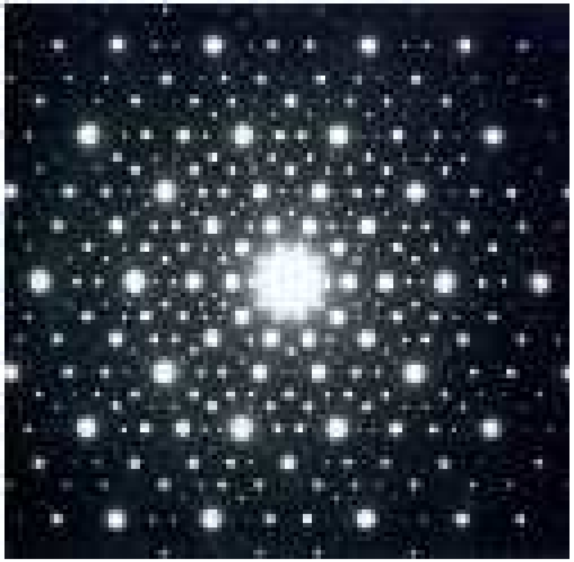
Part I.

1. **Basic icosahedral tilings**
2. Point substitution processes

Part II.

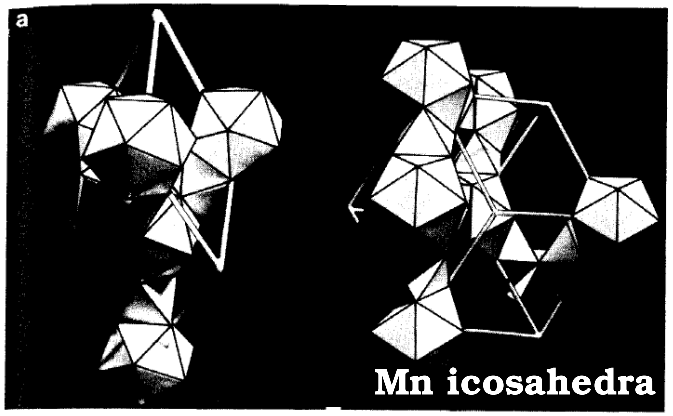
3. Tilings constructed with PIRs
4. Canonical cell tilings
5. Toward icosahedral CCTs

Icosahedral QCs



ED pattern along 5-fold axis of an icosahedral quasicrystal

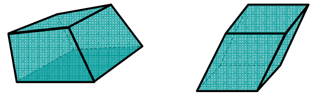
Icosahedral tilings



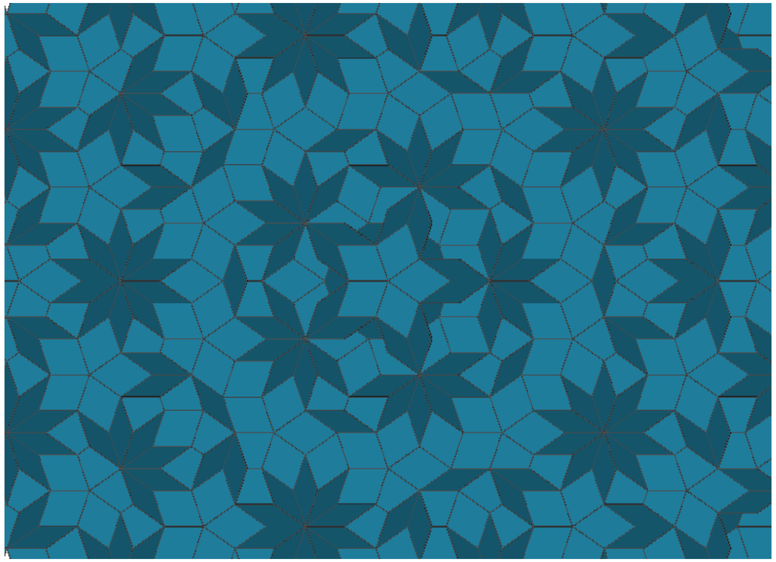
b-c packing of icosahedral clusters (F-type) based on the rhombohedral tiling (Ammann-Kramer tiling).

Model of *i* -(Al-Mn),
M. Audier and P. Guyot,
Phil. Mag. B 53, L43 (1986)

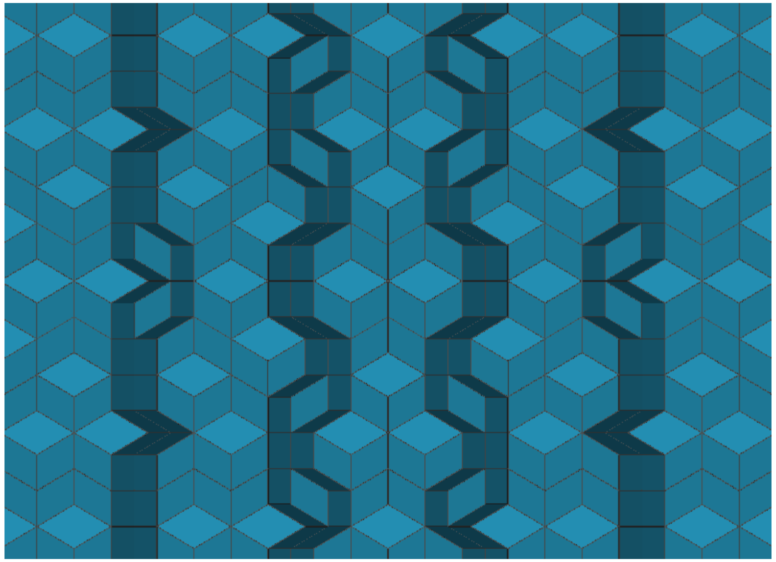
$\mathcal{T}^{*(P)}$ tiling (Ammann-Kramer tiling)



Basic tiles OR, AR
(Ammann rhombohedra)



5-fold view

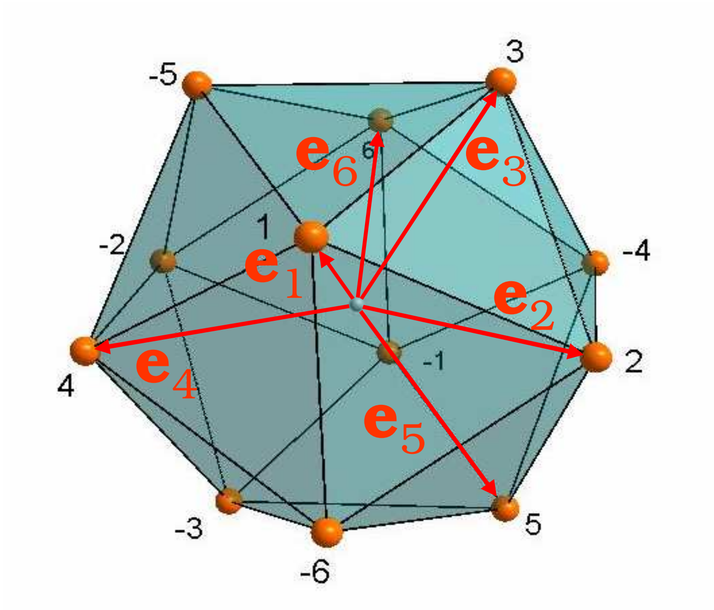


2-fold view

M. Duneau and A. Katz, Phys. Rev. Lett. 54, 2688 (1985).
P. Kramer and R. Neri, Acta Cryst. A 40, 580 (1984).

Icosahedral basis set

$$\begin{pmatrix}\mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 & \mathbf{e}_4 & \mathbf{e}_5 & \mathbf{e}_6\end{pmatrix} = \begin{pmatrix} \tau & 0 & 1 & 1 & -\tau & 0 \\ 1 & \tau & 0 & 0 & 1 & -\tau \\ 0 & 1 & \tau & -\tau & 0 & 1 \end{pmatrix}$$



$$\| \mathbf{e}_1 \| = \sqrt{2+\tau}$$

$$\tau = \frac{1+\sqrt{5}}{2}$$

the golden mean

Icosahedral modules

$$\mathbf{M}_P := \{n_1\mathbf{e}_1 + n_2\mathbf{e}_2 + n_3\mathbf{e}_3 + n_4\mathbf{e}_4 + n_5\mathbf{e}_5 + n_6\mathbf{e}_6 \mid (n_j) \in Z^6\}$$

$Z[\tau^3]$

$$\mathbf{M}_F := \{n_1\mathbf{e}_1 + n_2\mathbf{e}_2 + n_3\mathbf{e}_3 + n_4\mathbf{e}_4 + n_5\mathbf{e}_5 + n_6\mathbf{e}_6 \mid \sum_j n_j = 0 \bmod 2, (n_j) \in Z^6\}$$

$Z[\tau]$

$$\mathbf{M}_I := \{\nu_1\mathbf{e}_1 + \nu_2\mathbf{e}_2 + \nu_3\mathbf{e}_3 + \nu_4\mathbf{e}_4 + \nu_5\mathbf{e}_5 + \nu_6\mathbf{e}_6 \mid (\nu_j) \in Z^6 \cup Z^6 + \frac{1}{2}(111111)\}$$

$Z[\tau]$

integer ring

[1] T. Janssen, Acta Cryst. A 42 (1986) 261.

[2] D. S. Rokhsar *et al.*, Phys. Rev. B 35 (1987) 5487.

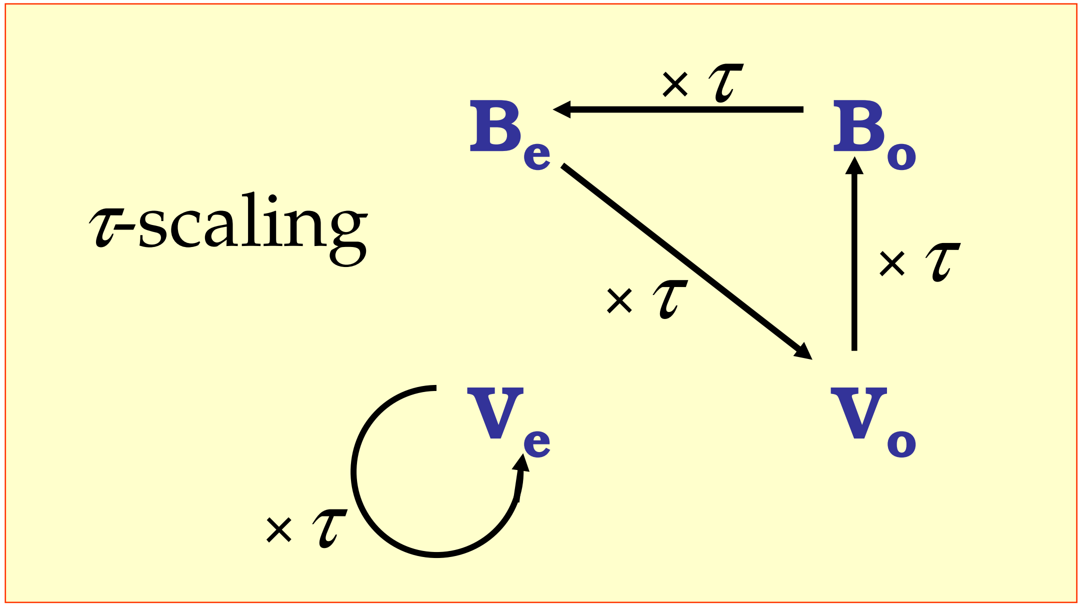
[3] L.S. Levitov and J. Rhyner, J. Physique 49 (1988) 1835.

Scale invariance of the modules

$$\mathbf{M}_I := \mathbf{M}_P \cup \left[\mathbf{M}_P + \frac{1}{2}(111111) \right]$$

$$= \mathbf{M}_F \cup [\mathbf{M}_F + (100000)] \cup \left[\mathbf{M}_F + \frac{1}{2}(\bar{1}11111) \right] \cup \left[\mathbf{M}_F + \frac{1}{2}(111111) \right]$$

$\downarrow$ $\mathbf{V_e}$ $\downarrow$ $\mathbf{V_o}$ $\downarrow$ $\mathbf{B_e}$ $\downarrow$ $\mathbf{B_o}$

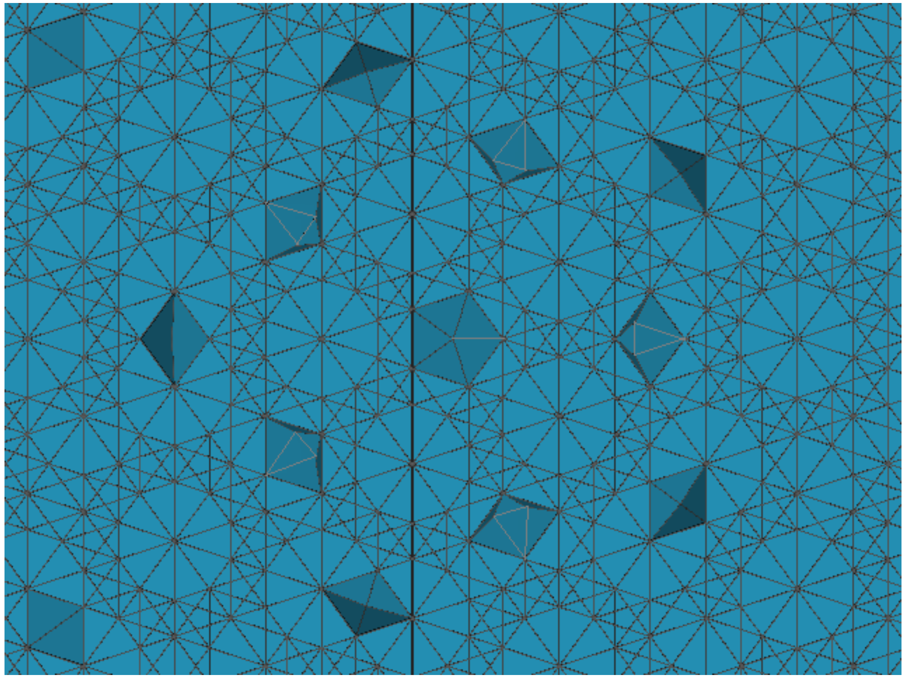


$$\mathbf{M}_P \times \tau^3 = \mathbf{M}_P$$

$$\mathbf{M}_F \times \tau = \mathbf{M}_F$$

$$\mathbf{M}_I \times \tau = \mathbf{M}_I$$

$\mathcal{T}^{*(2F)}$ tiling
(Kramer et al.)



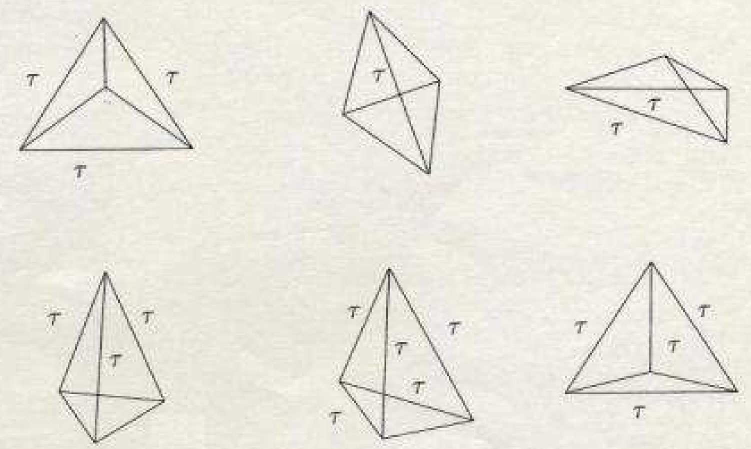


Fig. 4.22. *Top*: the triacontahedral vertex window $V_\perp \in E_\perp$ of the tiling $(\mathcal{T}^*, D_6)$. The holes a, c are marked by *black* and *white circles*. *Bottom*: the six tetrahedral tiles of the tiling in the order $(F^*, B^*, D^*; G^*, A^*, C^*)_\parallel \in E_\parallel$. The symbol τ denotes edges of length τ②

P. Kramer et al., in Symmetries in Science V: Algebraic Structures, their Representions, Realizations and Physical Applications, Ed. by B. Gruber *et al.*, Plenum Press, New York, 1991, pp. 395.

Outline

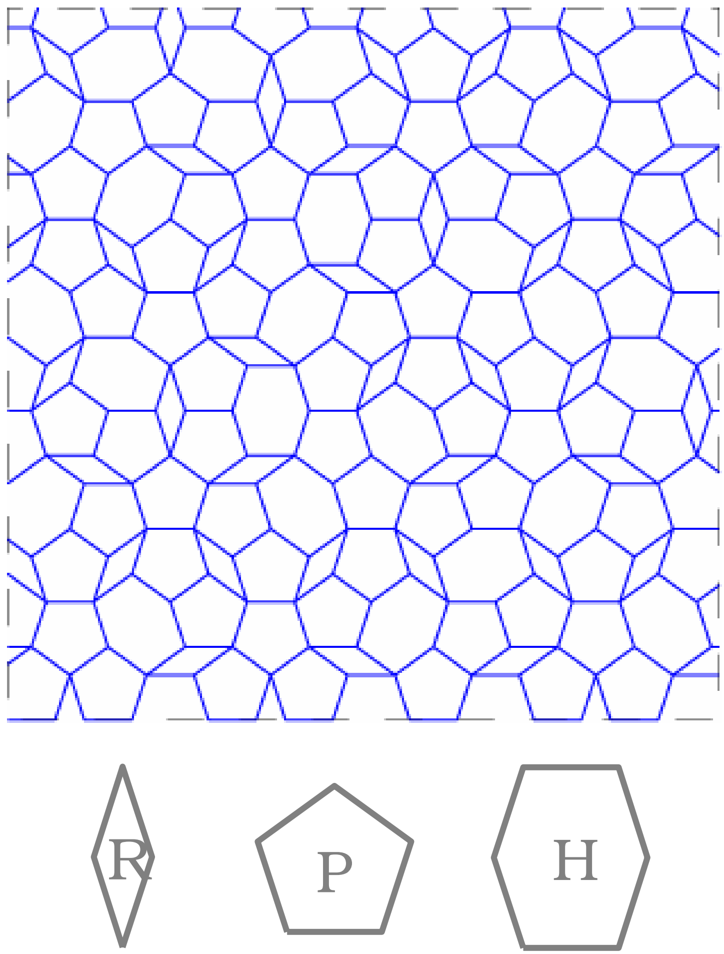
Part I.

1. Basic icosahedral tilings
2. **Point substitution processes**

Part II.

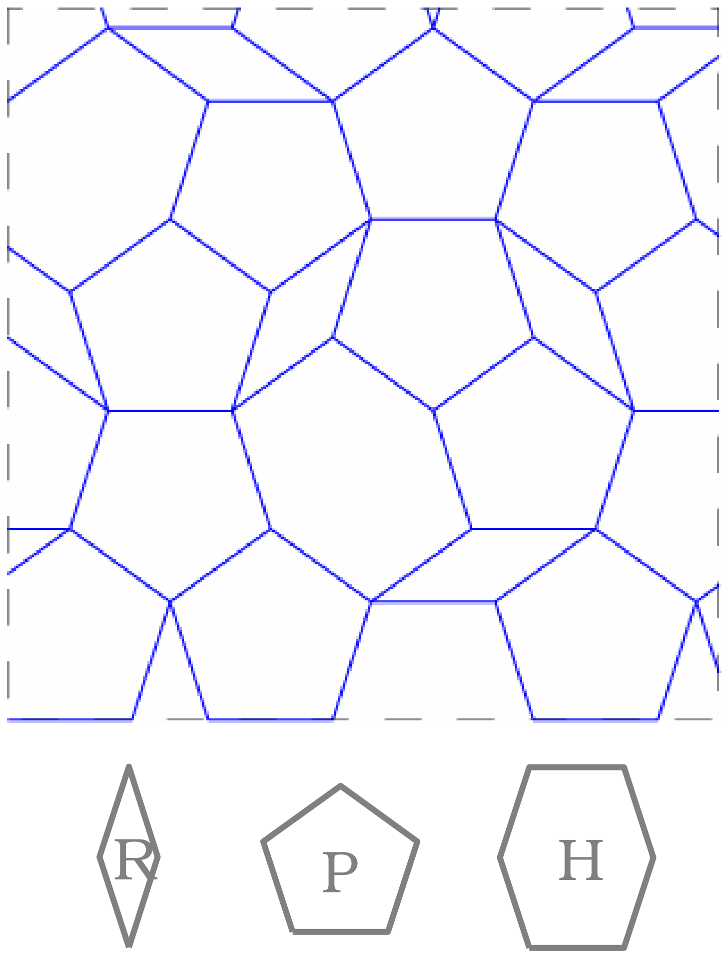
3. Tilings constructed with PIRs
4. Canonical cell tilings
5. Toward icosahedral CCTs

Point substitution processes for decagonal tilings



N. Fujita, Acta Cryst. A 65, 342 (2009)

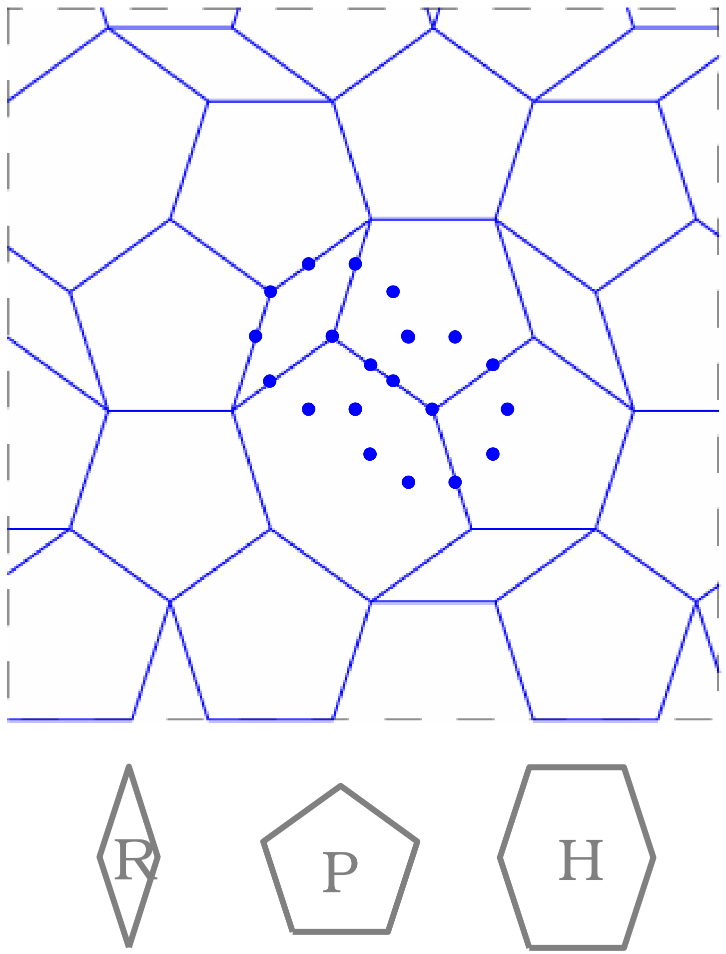
Point substitution processes for decagonal tilings



(1)Expansion
($\sigma = \tau^2$)

N. Fujita, Acta Cryst. A 65, 342 (2009)

Point substitution processes for decagonal tilings

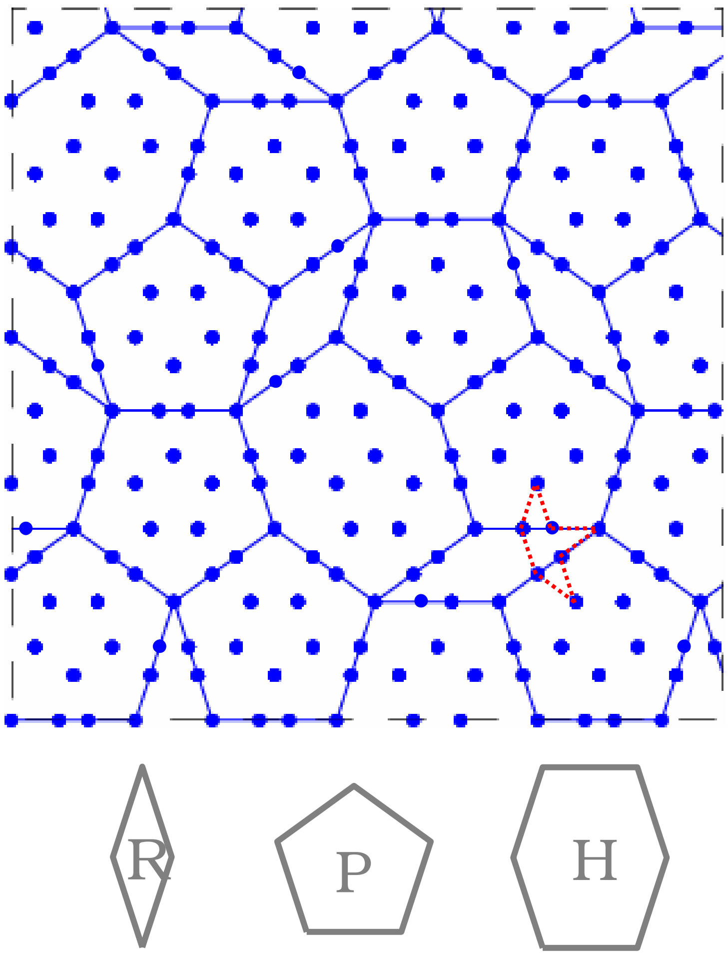


(1)Expansion
($\sigma = \tau^2$)

(2)Place **S** at
every vertex

N. Fujita, Acta Cryst. A 65, 342 (2009)

Point substitution processes for decagonal tilings

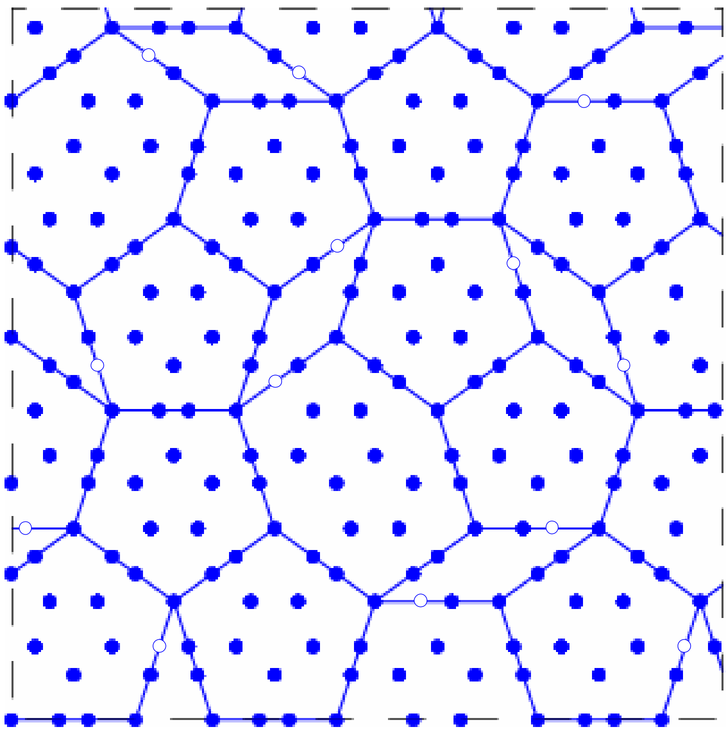


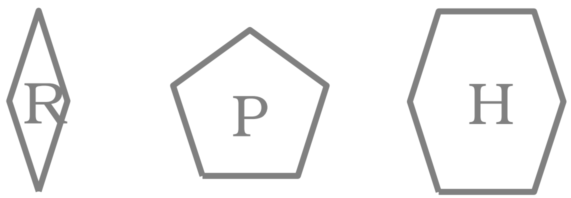
(1)Expansion
($\sigma=\tau^2$)

(2)Place **S** at every vertex

N. Fujita, Acta Cryst. A 65, 342 (2009)

Point substitution processes for decagonal tilings





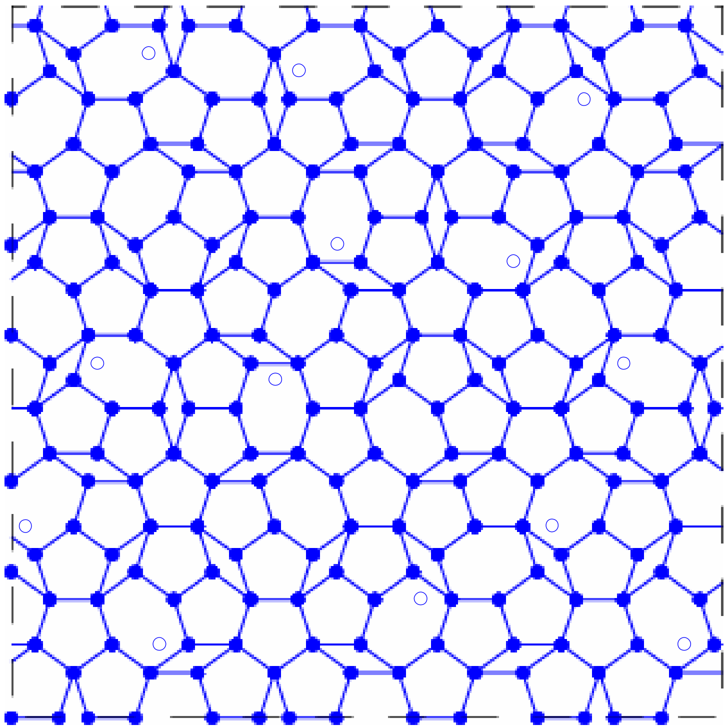
(1)Expansion
($\sigma=\tau^2$)

(2)Place **S** at every vertex

(3)Eliminate excessive points

N. Fujita, Acta Cryst. A 65, 342 (2009)

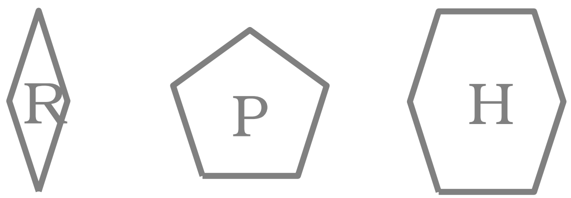
Point substitution processes for decagonal tilings



(1)Expansion
($\sigma = \tau^2$)

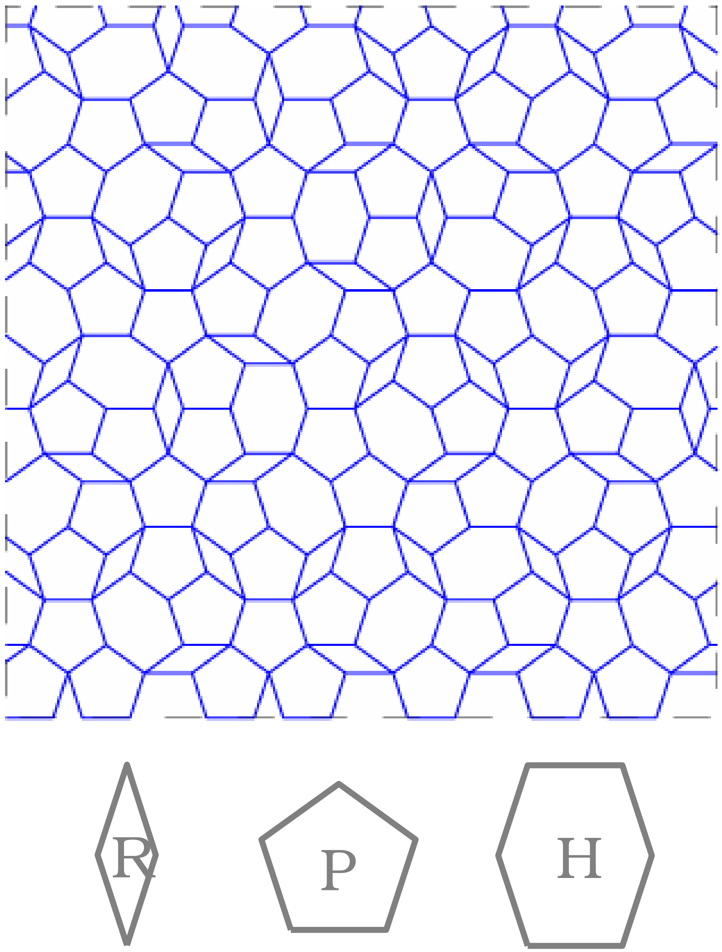
(2)Place **S** at every vertex

(3)Eliminate excessive points



N. Fujita, Acta Cryst. A 65, 342 (2009)

Point substitution processes for decagonal tilings

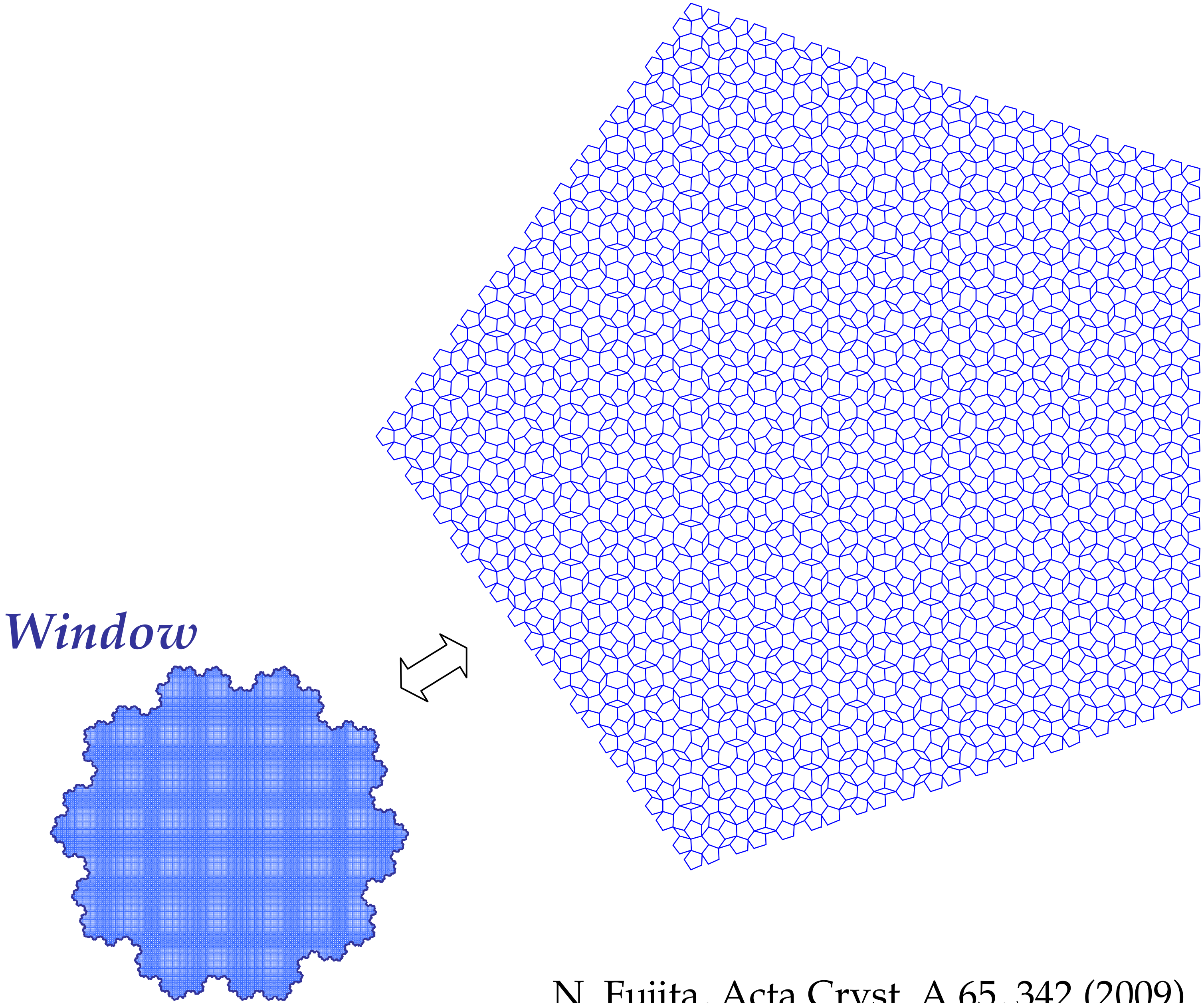


(1)Expansion
($\sigma = \tau^2$)

(2)Place **S** at every vertex

(3)Eliminate excessive points

N. Fujita, Acta Cryst. A 65, 342 (2009)



N. Fujita, Acta Cryst. A 65, 342 (2009)

Point Substitution Process

(for constructing icosahedral quasiperiodic tilings)

(1)Expansive similarity transformation:

$\mathbf{T}_i \rightarrow \sigma \mathbf{T}_i$ ($\mathbf{T}_i \subset \mathbf{M}$, $\sigma = \rho^n$, $\rho = \tau^3$(P), τ(F), τ(I))

(2) Replicate the I_h-star at every vertex:

$\mathbf{T}_i' = \sigma \mathbf{T}_i + \mathbf{S}$ ($\mathbf{S} \subset \mathbf{M}$)

(3) Decimation of points by local rules:

$\mathbf{T}_i' \rightarrow \mathbf{T}_{i+1}$ ($\subset \mathbf{T}_i'$)

N. Fujita, Acta Cryst. A 65, 342 (2009)

Step (3) is needed if there is redundancy in the points generated through (1) and (2) (→Point inflation rule)

K. Niizeki, J.Phys.A:Math.Theor.41,175208 (2008)

Outline

Part I.

1. Basic icosahedral tilings
2. Point substitution processes

Part II.

3. **Tilings constructed with PIRs**
4. Canonical cell tilings
5. Toward icosahedral CCTs

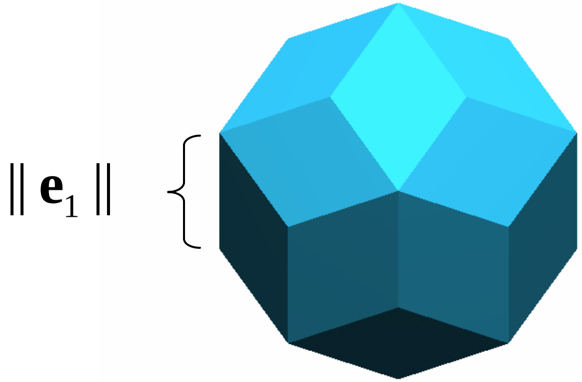
Windows

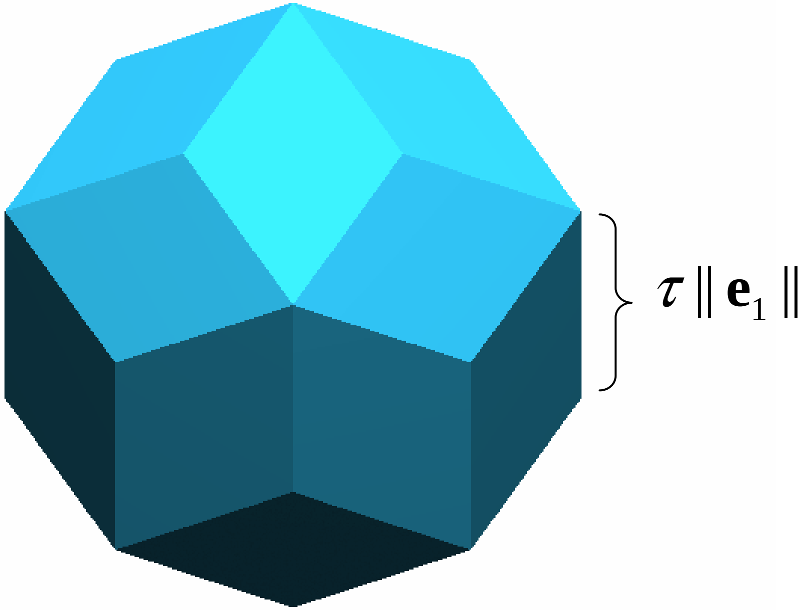
$\mathcal{T}^{*(\mathrm{P})}$

P-type

$\mathcal{T}^{*(\mathrm{2F})}$

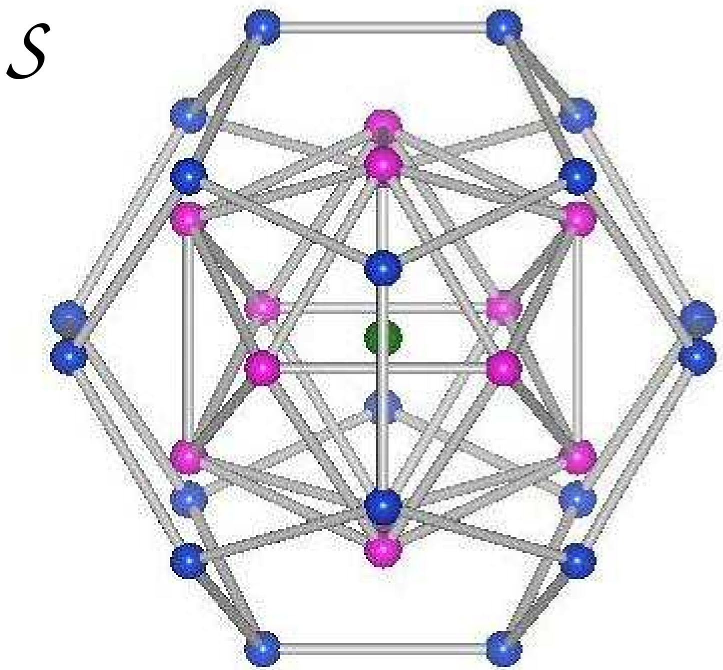
F-type





Point density $\dfrac{W_P}{\Omega_P}$ $\dfrac{W_F}{\Omega_F} = \dfrac{\tau^3}{2} \dfrac{W_P}{\Omega_P}$

I_h-star

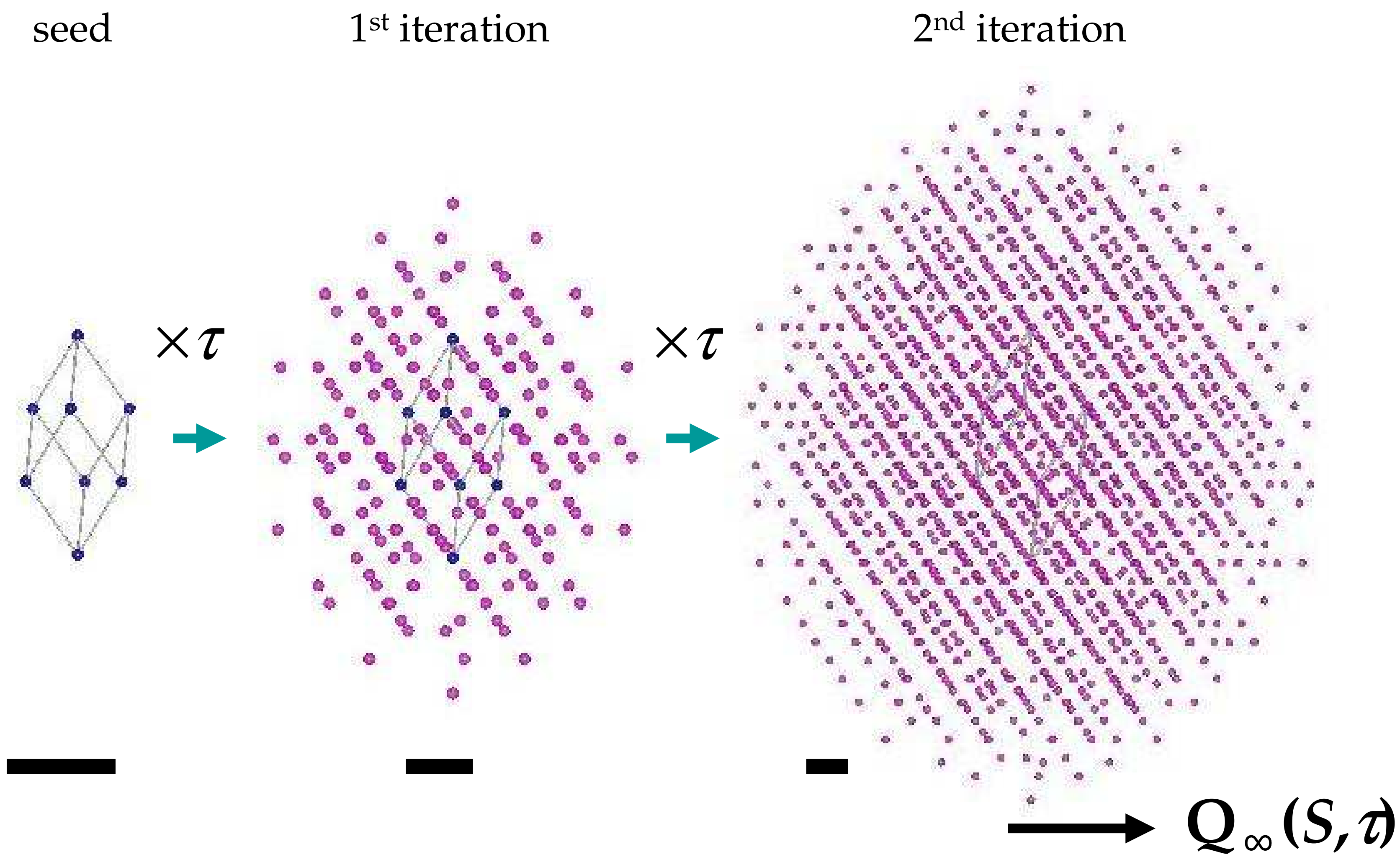


$1: (000000)$

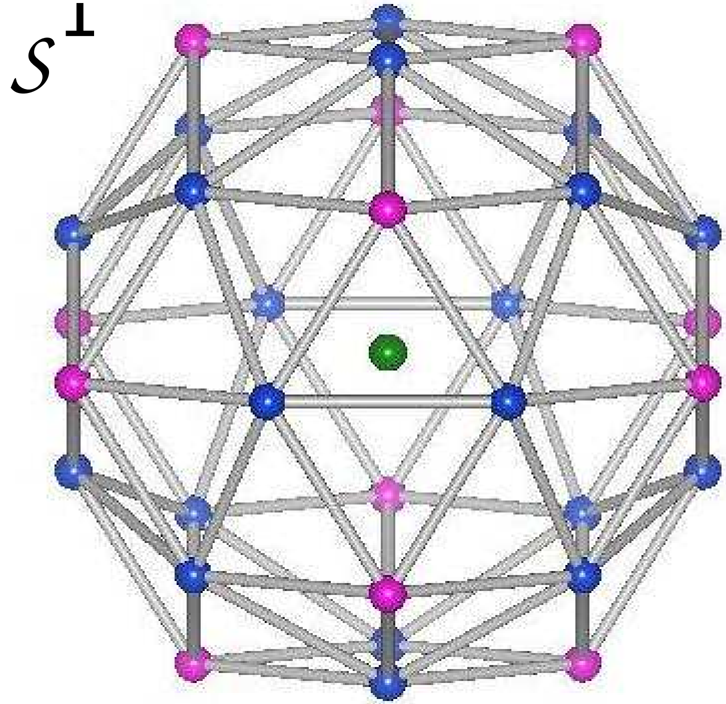
$2: \frac{1}{2}(1\,\bar{1}\,\bar{1}\,1\,\bar{1}\,\bar{1})$

$3: (111000)$

Point inflation rule
(viewed in the external space)



I_h-star
(mapped to the internal space)

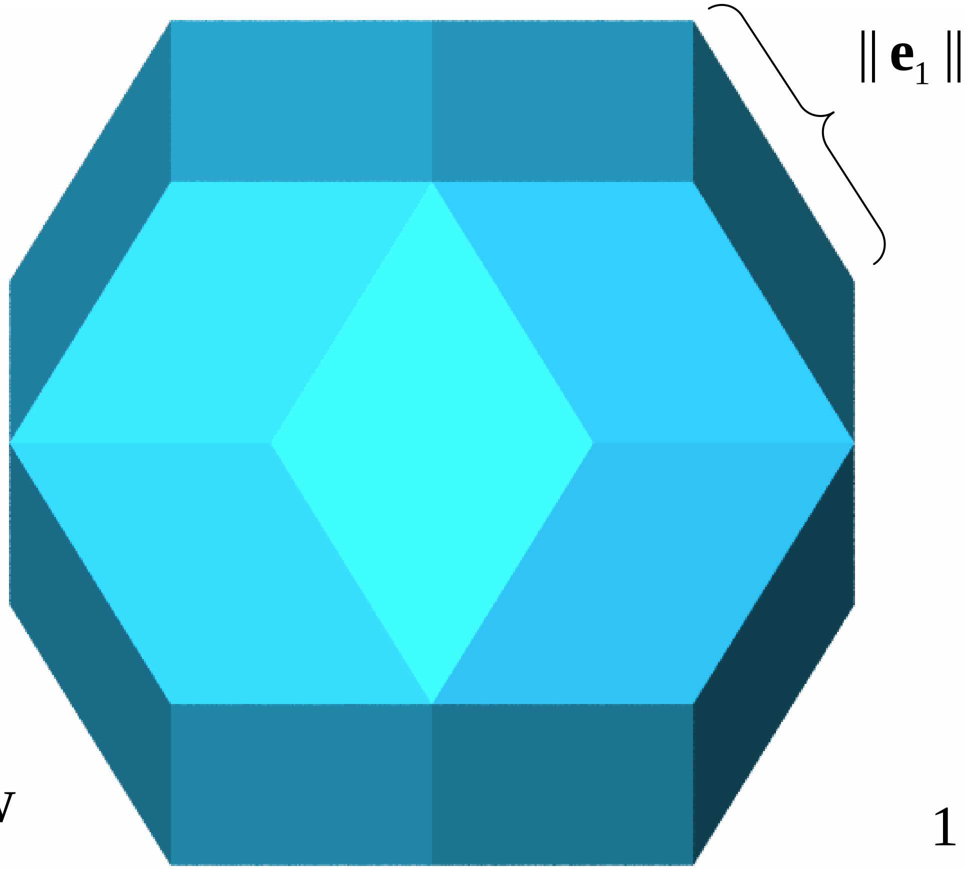


$1:(000000)$

$2:\frac{1}{2}(1\,\bar{1}\,\bar{1}\,1\,\bar{1}\,\bar{1})$

$3:(111000)$

in the internal space



window

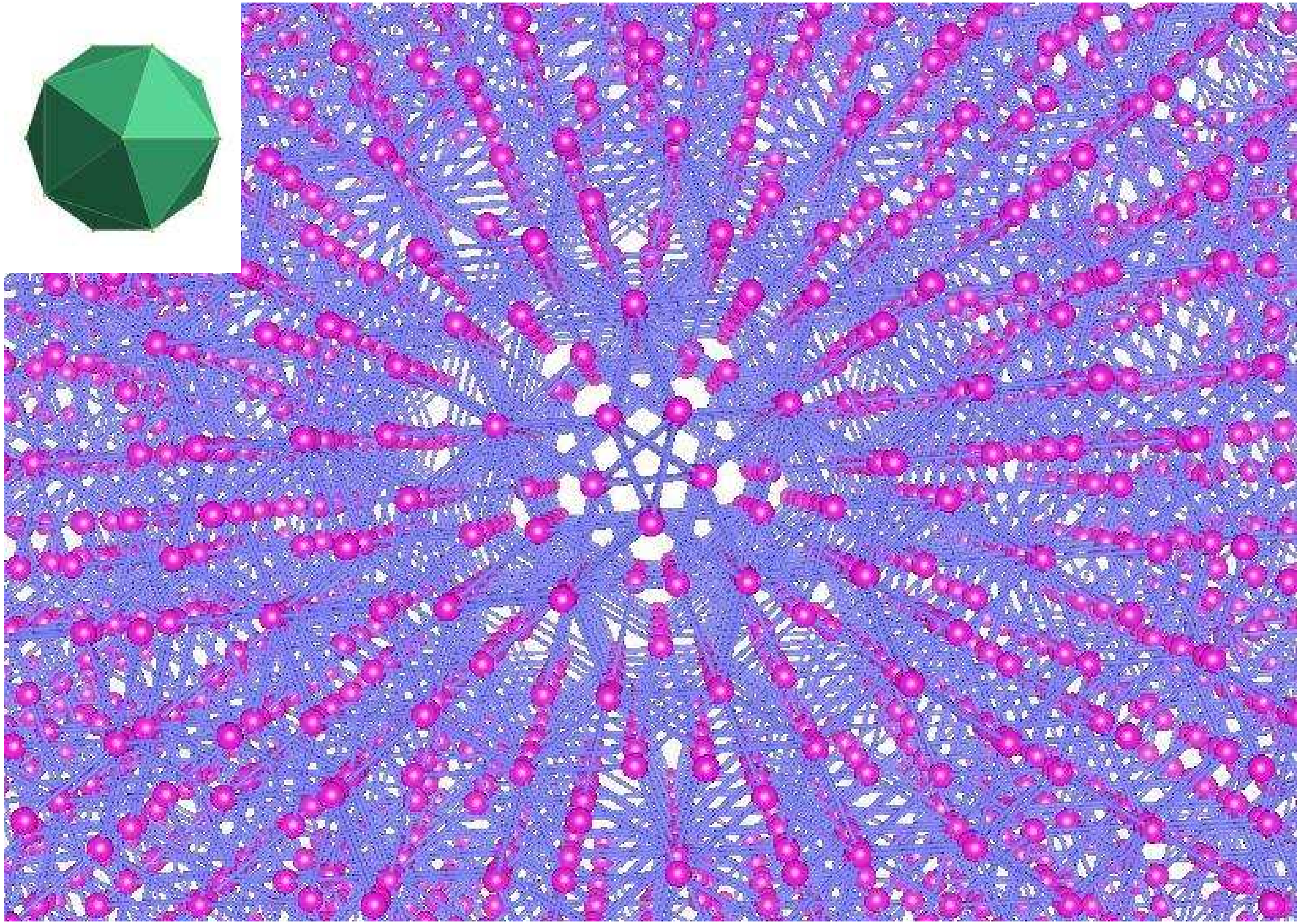
$$1: (000000)$$

$$2: \frac{1}{2}(1\,\bar{1}\,\bar{1}\,1\,\bar{1}\,\bar{1})$$

$$3: (111000)$$

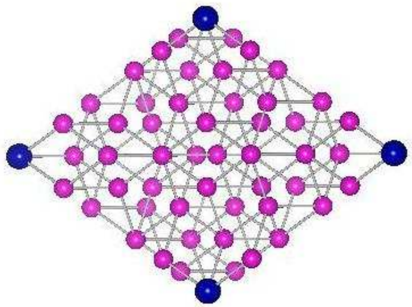
$$1+\tau^{-1}+\tau^{-2}+\tau^{-3}+\tau^{-4}+\tau^{-5}+\cdots=\frac{1}{1-\tau^{-1}}=\tau^{2}=2.61803$$

5-fold direction



$\mathbf{Q}_{\infty}(S, \tau) \cap \mathbf{M}_{\mathrm{P}}$

Inflation rule of the Ammann-Kramer tiling



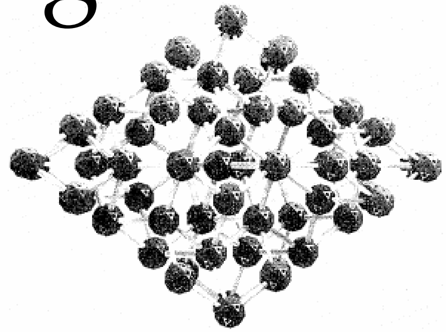
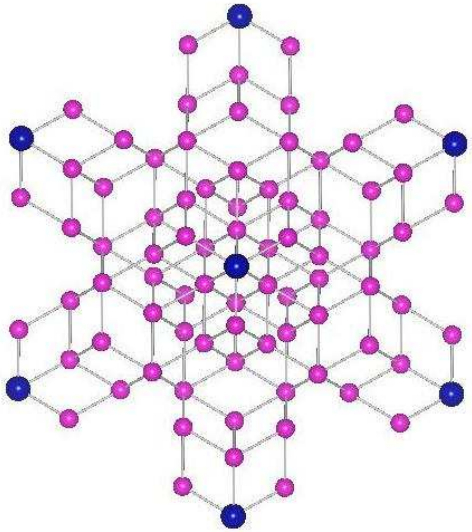


Fig. 1. The skeleton of an expanded A_6, view along a pentagonal axis.



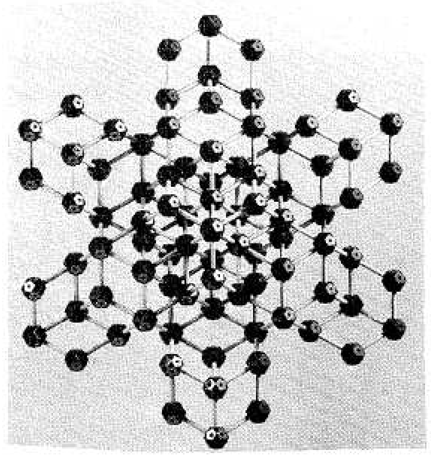


Fig. 2. The skeleton of an expanded O_6, view along a trigonal axis.

Inflation rules by τ^3 scaling

T. Ogawa, J. Phys. Soc. Jpn. 54, 3205 (1985).

Outline

Part I.

1. Basic icosahedral tilings
2. Point substitution processes

Part II.

3. Tilings constructed with PIRs
4. **Canonical cell tilings**
5. Toward icosahedral CCTs

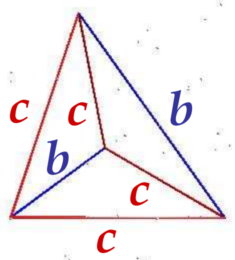
Canonical cell tiling

'Cell geometry for cluster-based quasicrystal models',

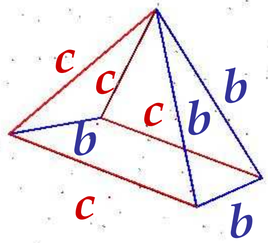
C. L. Henley, *Phys. Rev.* B 43 (1991) 993.

- 4 polyhedra: A-, B-, C-, D-cells

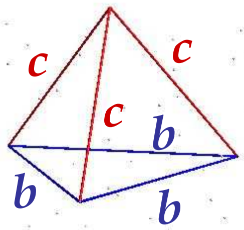
A-cell



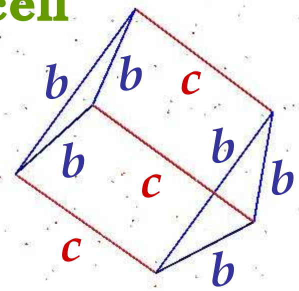
B-cell



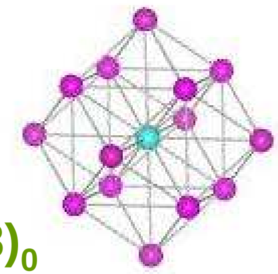
C-cell



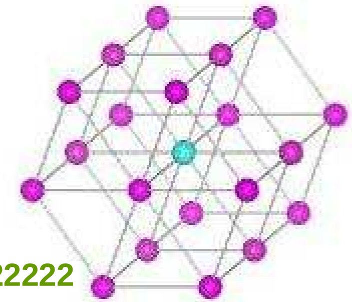
D-cell



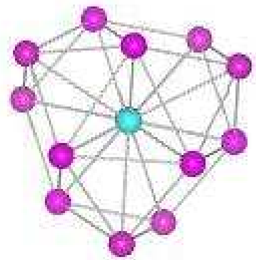
- There are 32 classes of nodes in a CCT



$(68)_0$

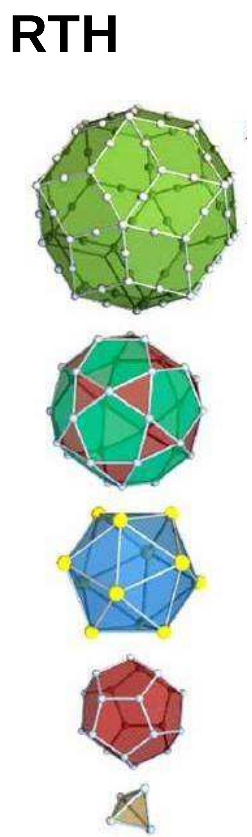


$(62)_{222222}$

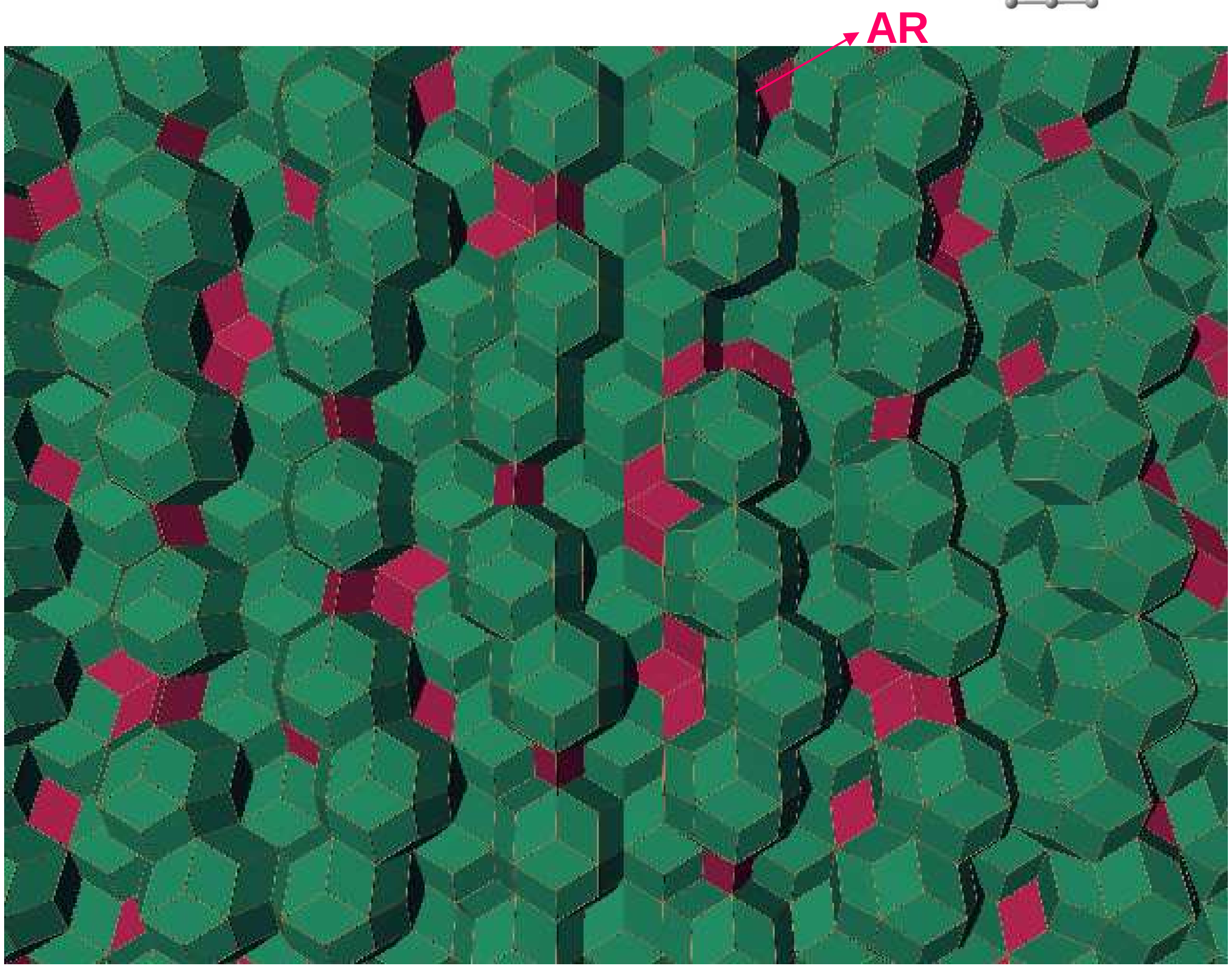


$(67)_{333}$

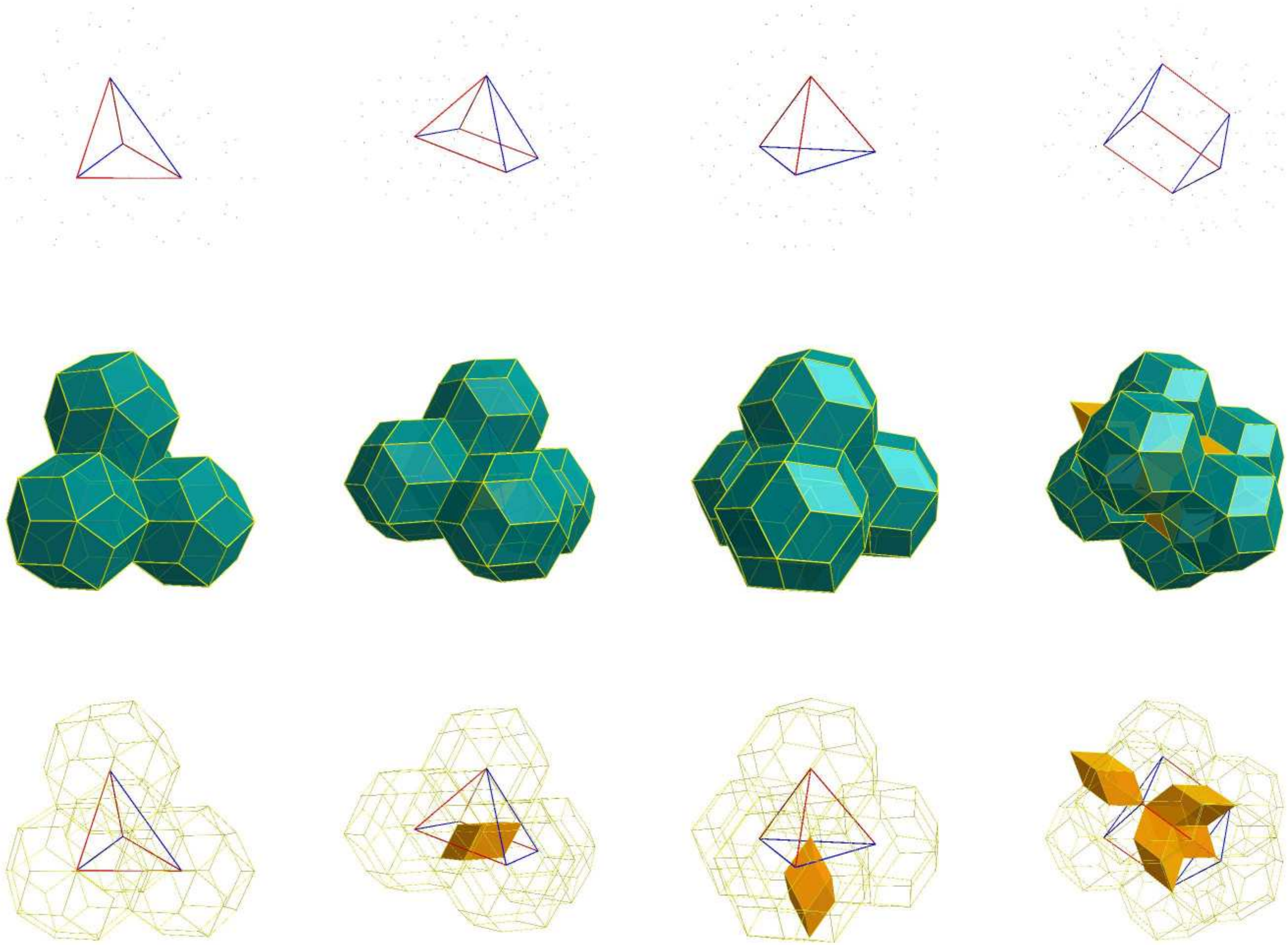
i-$Cd_{5.7}Yb$: Quasicrystal (QC)



H. Takakura & C.P. Gomez et al., (2007).



M. Mihalkovic et al., Phys. Rev. B 53, 9002-9020 (1996).



M. Mihalkovic et al., Phys. Rev. B 53, 9002-9020 (1996).

Outline

Part I.

1. Basic icosahedral tilings
2. Point substitution processes

Part II.

3. Tilings constructed with PIRs
4. Canonical cell tilings
5. **Toward icosahedral CCTs**

Is there an icosahedral CCT?

NO PROOF is given of the existence
of an ICOSAHEDRAL CCT

$\not\uparrow$

Methods to construct approximant CCTs
(under periodic boundary conditions)

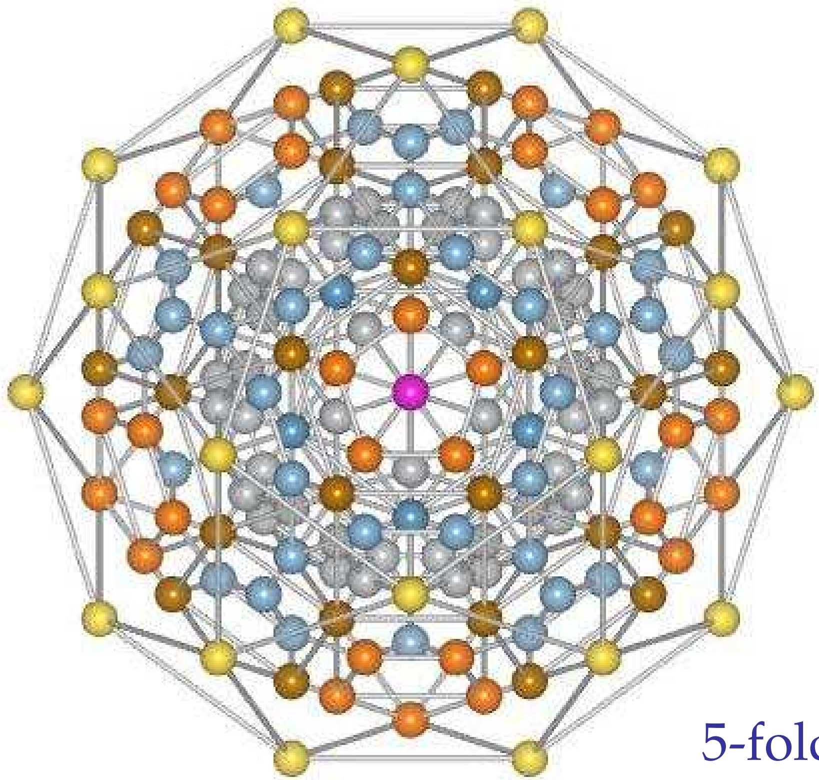
A Monte Carlo density optimization method:

M. Mihalkovic and P. Mrafko, *Europhys. Lett.* 21 (1993) 463.

A brute force algorithm:

M.E.J. Newman, C.L. Henley, and M. Oxborrow, *Phil. Mag. B* 71 (1995) 991.

Point sutstitution processes for icosahedral CCTs



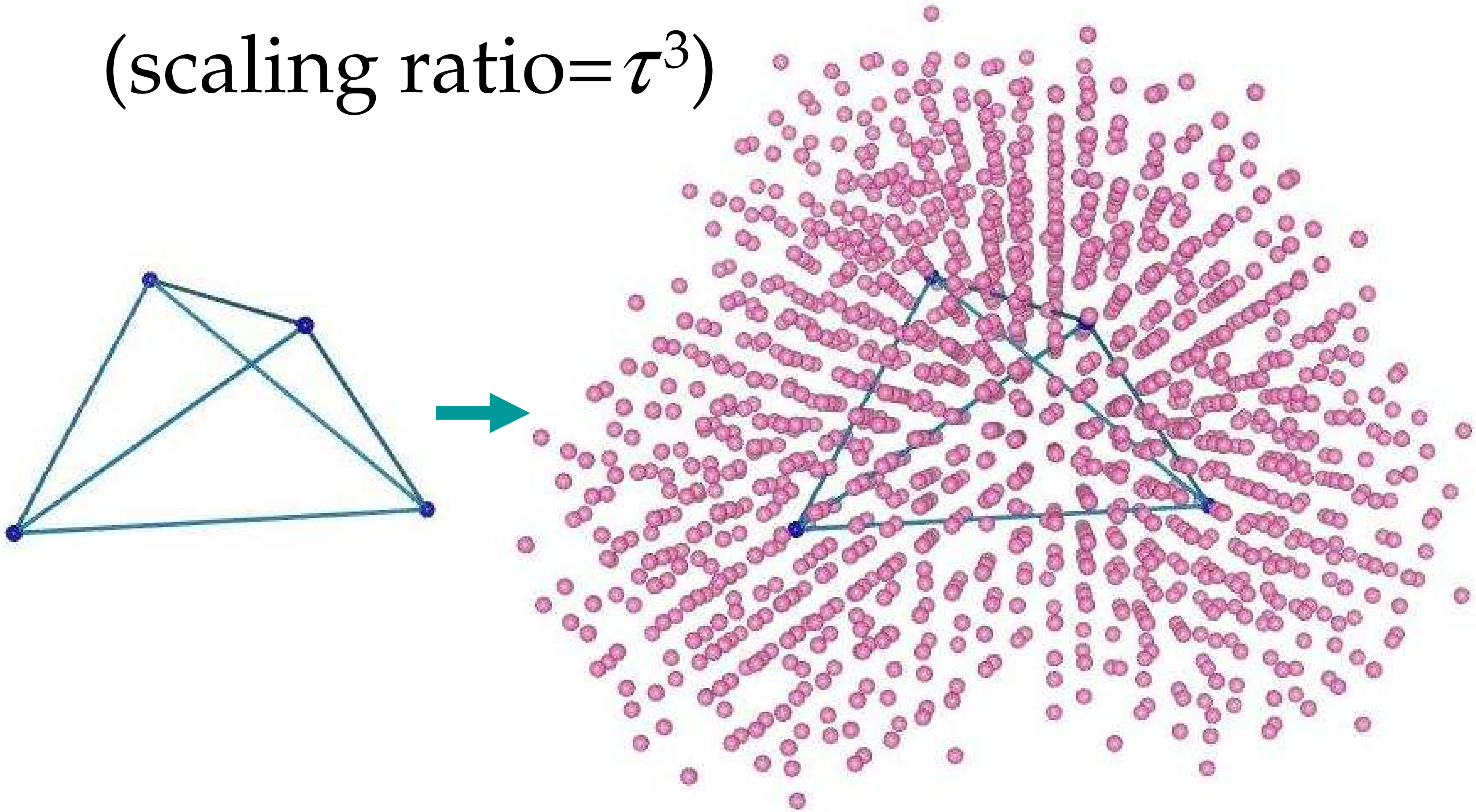
5-fold view

***I_h*-star**

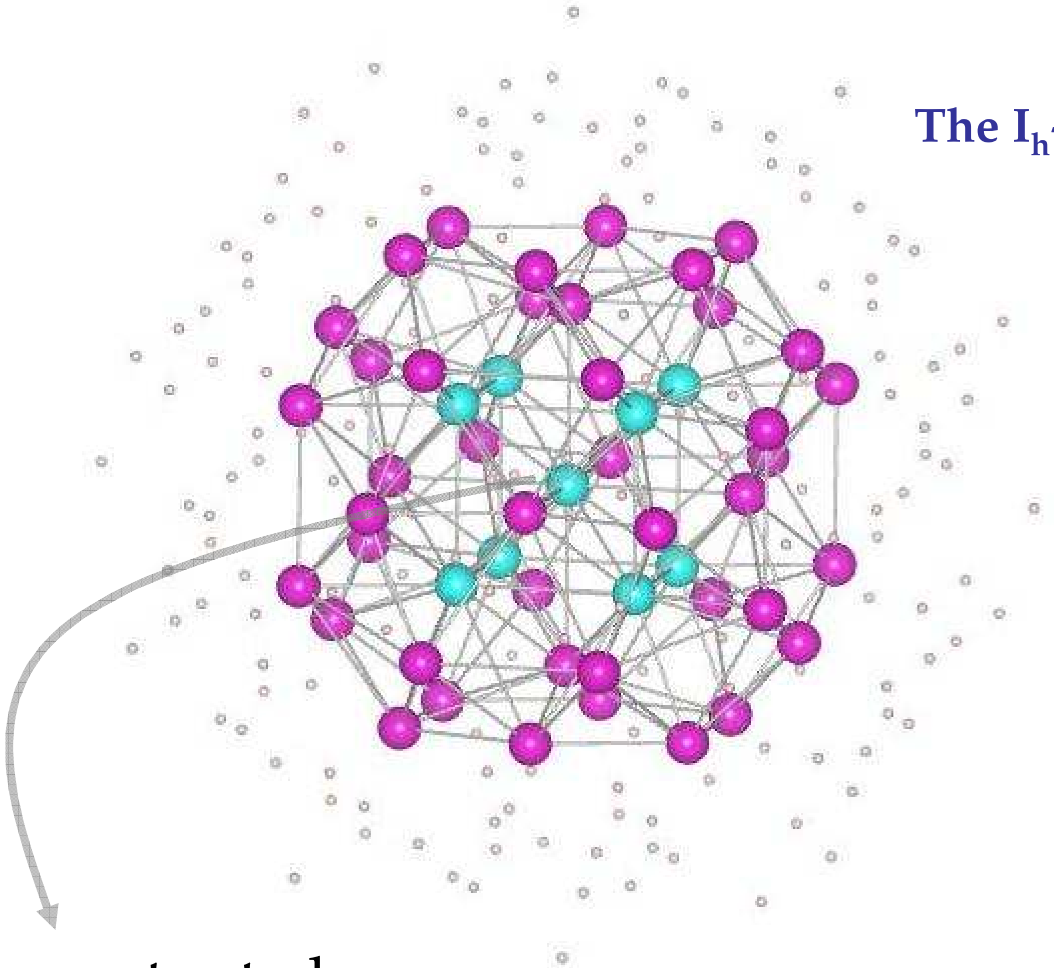
the magic star

The I_h-star is placed on every vertex of the expanded CCT

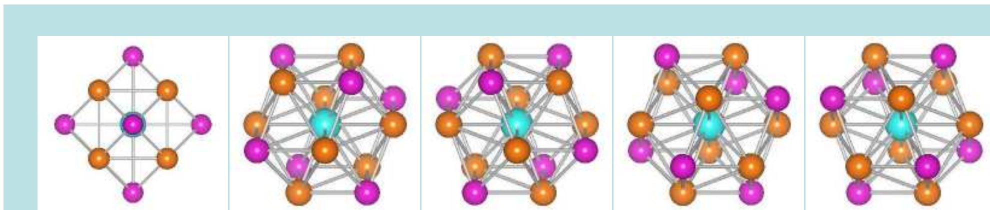
(scaling ratio= τ^3)



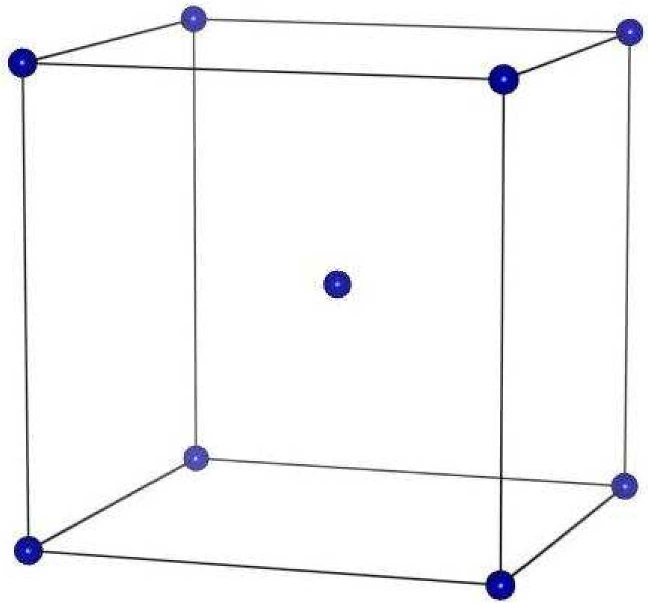
The I_h-star

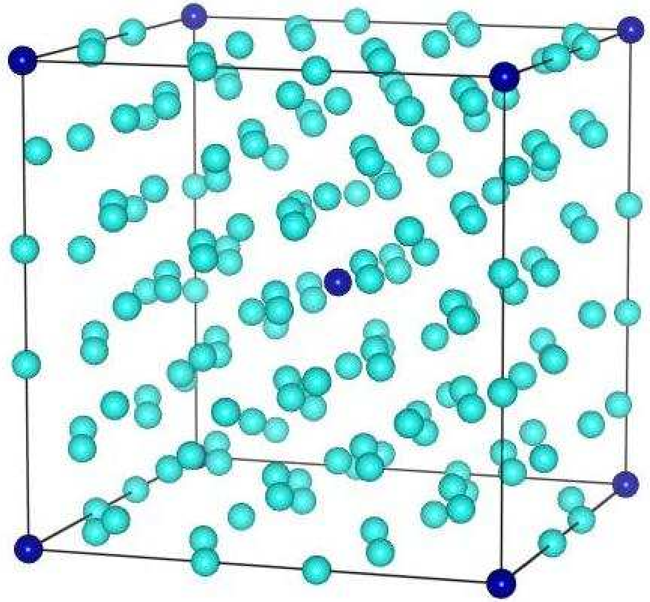


Fix the center to be the $(68)_0$ type node.



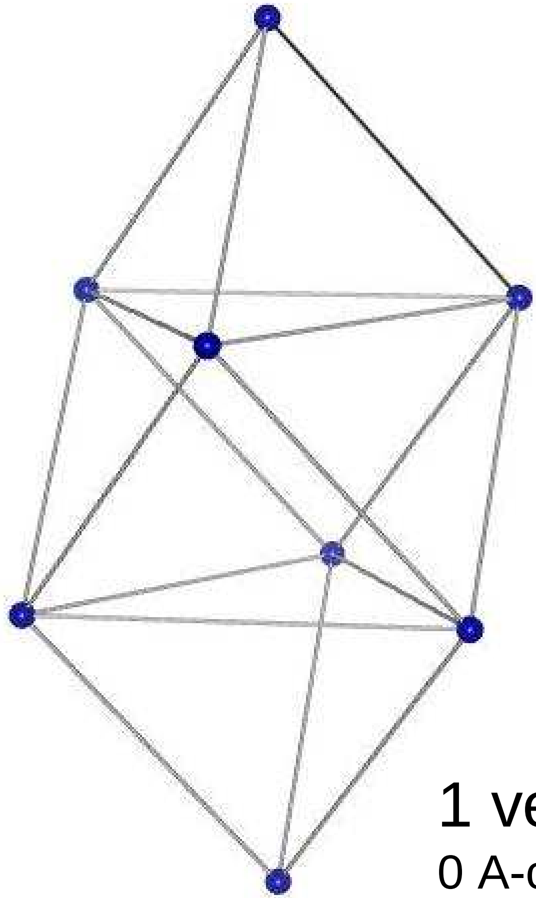
A-packing
(body centered cubic)



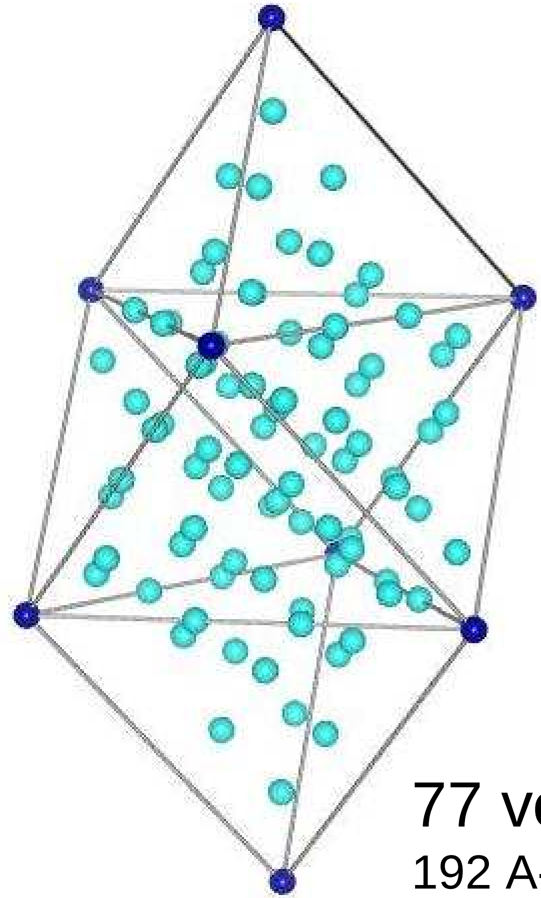


2 vertices	138 vertices
12 A-cells	348 A-cells
0 B-cell	136 B-cells
0 C-cell	136 C-cells
0 D-cell	24 D-cells

BC-packing (rhombohedral)



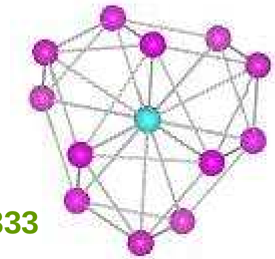
1 vertex
0 A-cell
2 B-cells
2 C-cells
0 D-cell



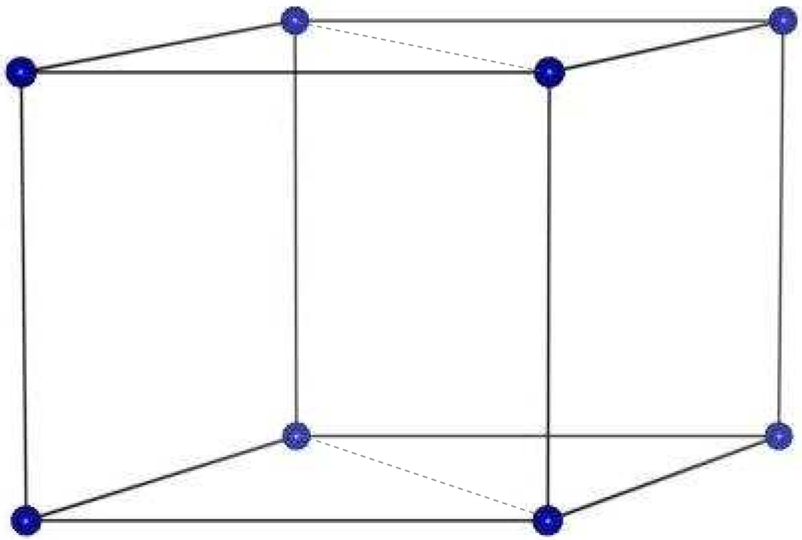
77 vertices
192 A-cells
76 B-cells
76 C-cells
14 D-cells

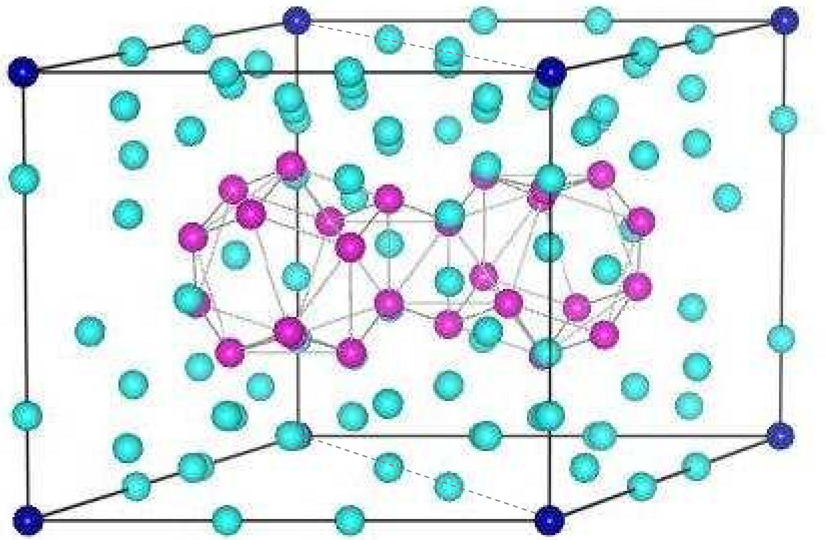
D-packing
(simple hexagonal)

$(67)_{333}$



The center is missing!





1 vertex

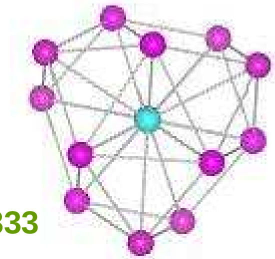
0 A-cells

0 B-cells

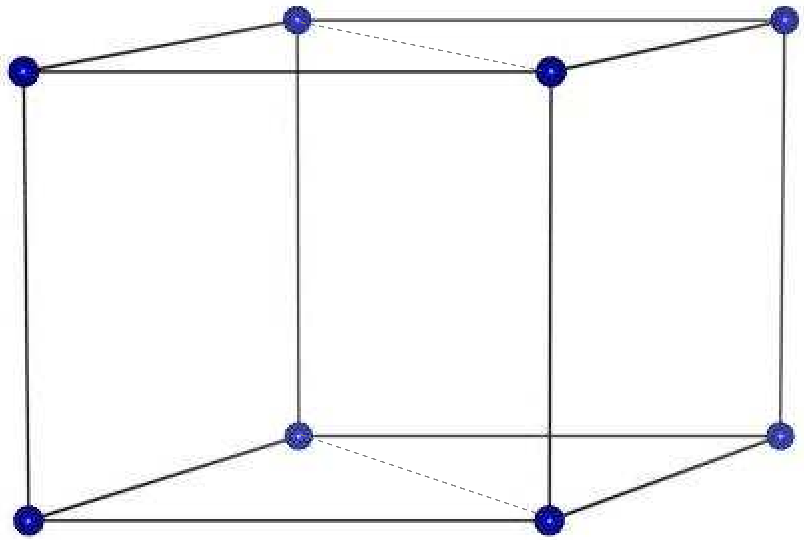
0 C-cells

2 D-cells

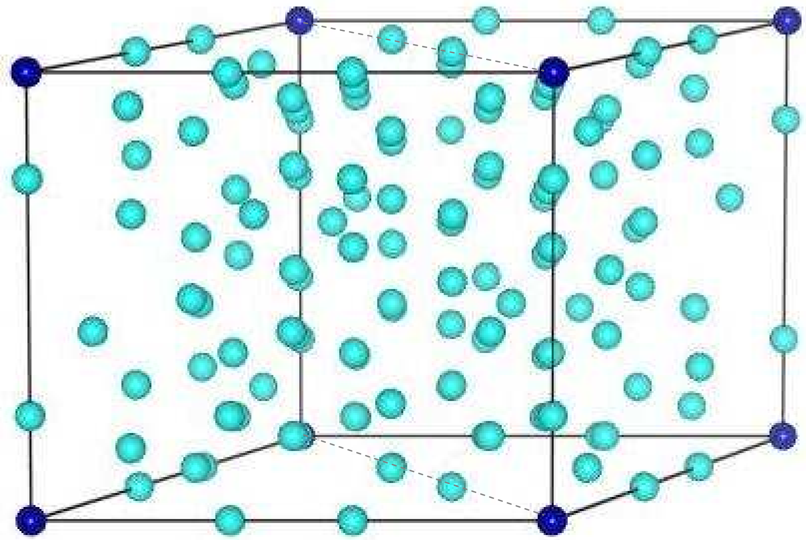
D-packing (simple hexagonal)



The center is missing!

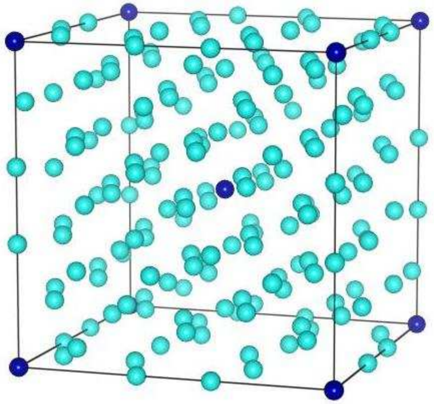


1 vertex
0 A-cells
0 B-cells
0 C-cells
2 D-cells



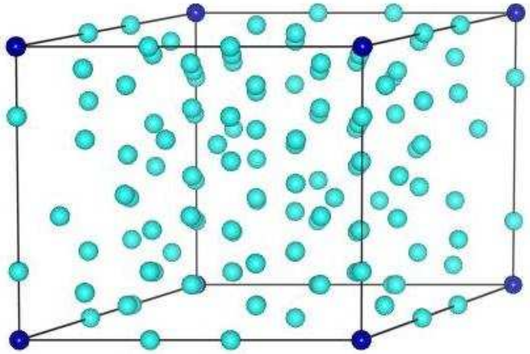
103 vertices
252 A-cells
102 B-cells
102 C-cells
20 D-cells

$\tau^3 \times$ A-packing



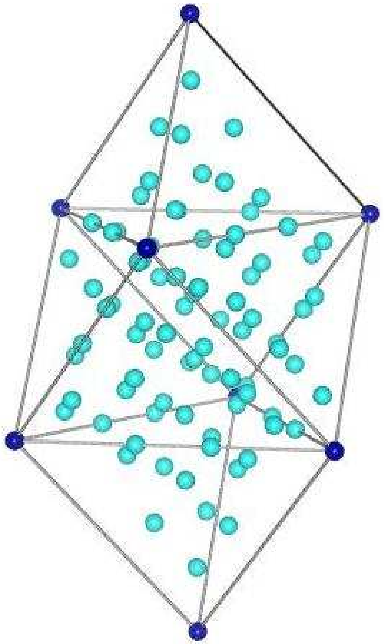
138 vertices
348 A-cells
136 B-cells
136 C-cells
24 D-cells

$\tau^3 \times$ D-packing



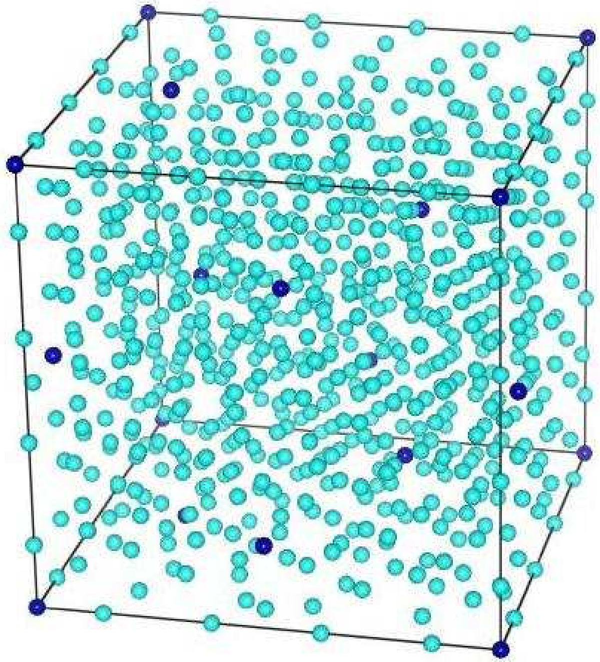
103 vertices
252 A-cells
102 B-cells
102 C-cells
20 D-cells

$\tau^3 \times$ BC-packing



77 vertices
192 A-cells
76 B-cells
76 C-cells
14 D-cells

$\tau^3 \times$ 2/1 cubic-packing



584 vertices
1464 A-cells
576 B-cells
576 C-cells
104 D-cells

Conclusion

The present scheme has turned out to be useful for constructing icosahedral tilings.

The magic star can generate all the vertices of an inflated CCT except a point in the center of each expanded D-cell.

It is likely that there exist τ^3-inflation rules for generating an icosahedral CCT, the proof of which still needs to be worked out.