Canonical-cell geometry: a renewed perspective

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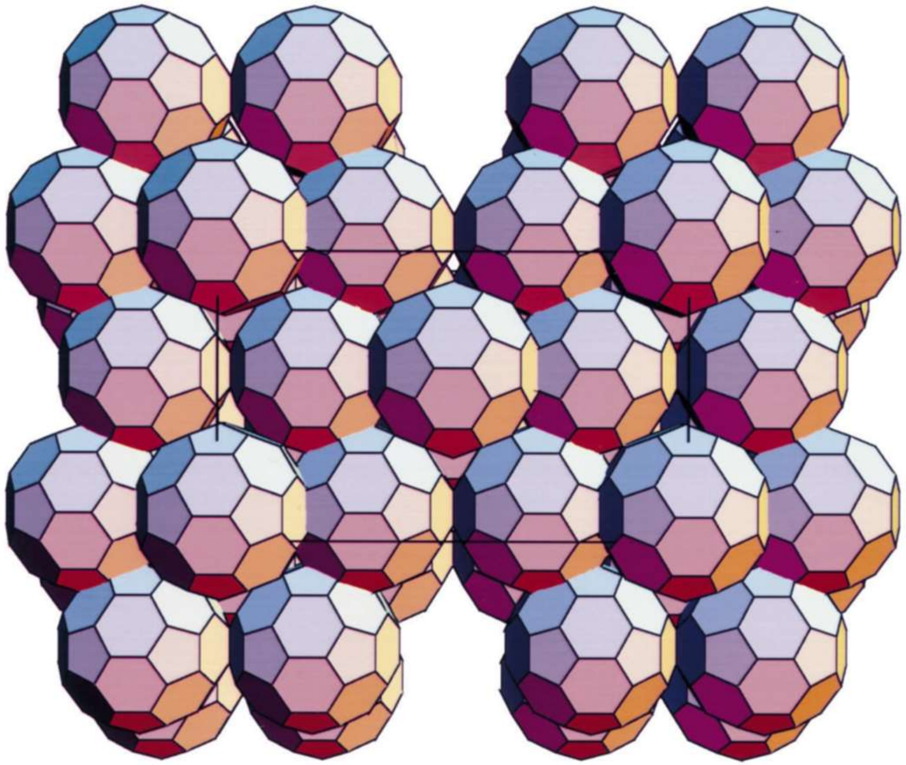
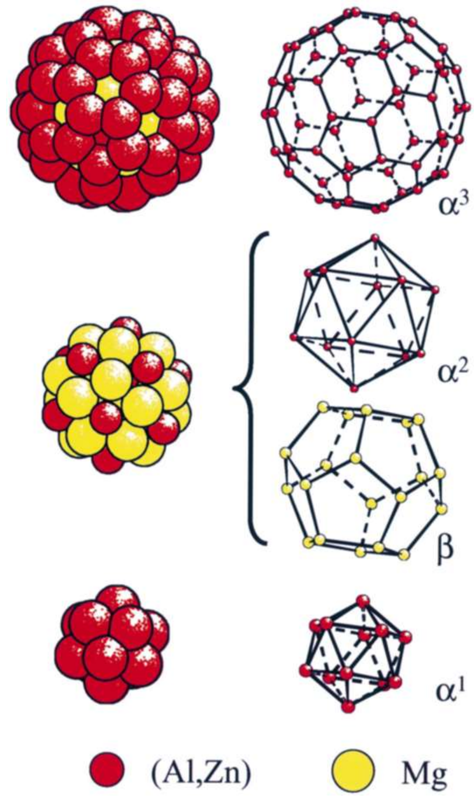
Packing of icosahedral clusters

S. G.
$Cmc2_1$



$(Ga,Zn)_{43}Mg_{26}$

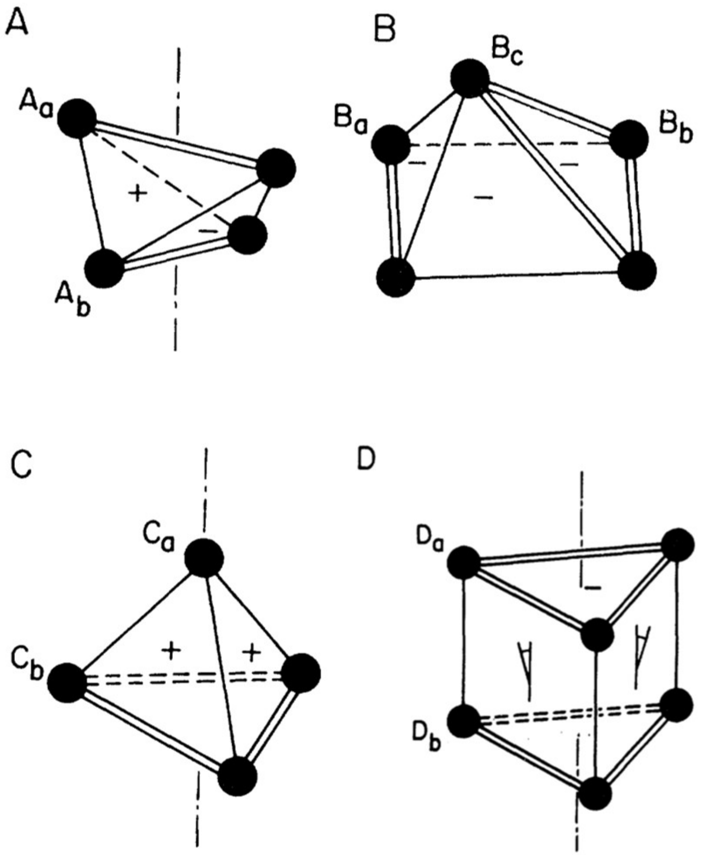
Bergman cluster



(104 atoms)

G. Kreiner, J. Alloys and Compd. 338 (2002) 261–273

Canonical cell tiling (CCT)



Prof. C. L. Henley (Cornell Univ.)
 - 2015

PHYSICAL REVIEW B VOLUME 43, NUMBER 1 1 JANUARY 1991

Cell geometry for cluster-based quasicrystal models

Christopher L. Henley
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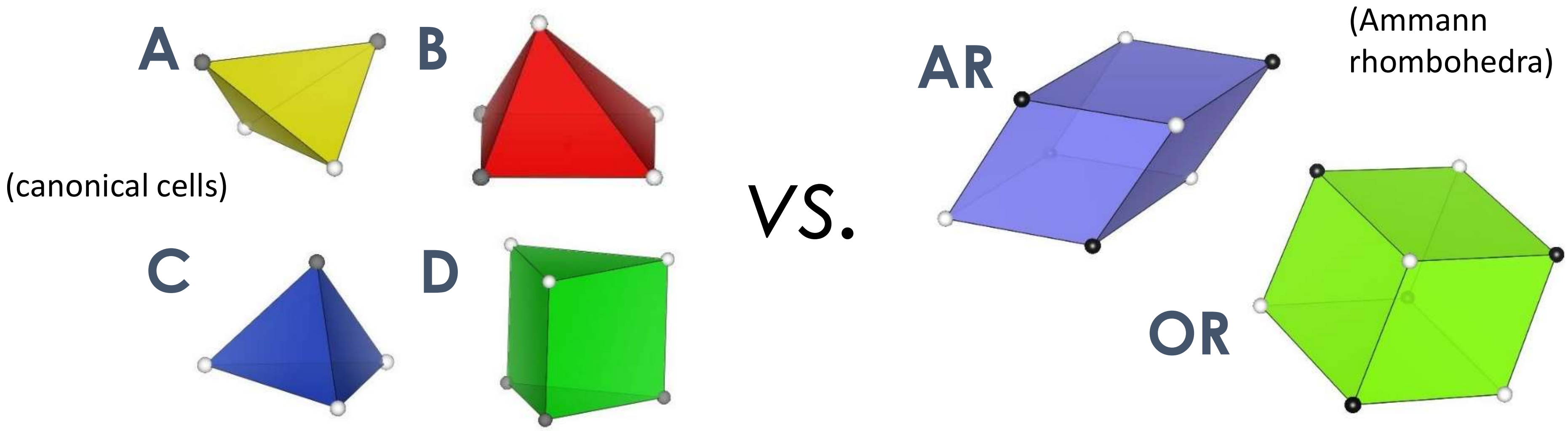
(Received 14 March 1990)

A new model of the geometrical structure of icosahedral quasicrystals is discussed that is based on icosahedral clusters connected by linkages (consistent with currently accepted motifs of the atomic structure), yet that is also a tiling by four kinds of "canonical cells." Such a geometry is convenient for complete atomic structure models defined by decoration, especially if configurational disorder is to be included. The canonical-cell tiling is related and compared with previous models such as packings of Ammann rhombohedra, sphere packings on Penrose tilings, and two decoration models of Audier. The frequency of occurrence is estimated for each kind of cell or other geometrical object—the basis for stoichiometry calculations of decoration models. The 32 distinct local environments around a given cluster are described. Many useful *periodic* tilings of this class are described providing useful "rational approximants" of the true structure and hypothetical structure models for some recently discovered approximant crystal phases.

Cell geometry for cluster-based quasicrystal models
C. L. Henley, *Phys. Rev. B* 43, 993 (1991).

CCT vs. 3DPT

- ✓More kinds of cell with less aesthetical shapes
- ✓More kinds of face (more complex matchings)
- ✓More difficulty in connecting it with the 6D scheme
- ✓Larger possibilities in arranging the cells
- ✓Less feasibility to construct a quasiperiodic tiling



Aim & Scope

Introduction to CCT

Geometry & Examples

Recent developments

Quasiperiodic CCT

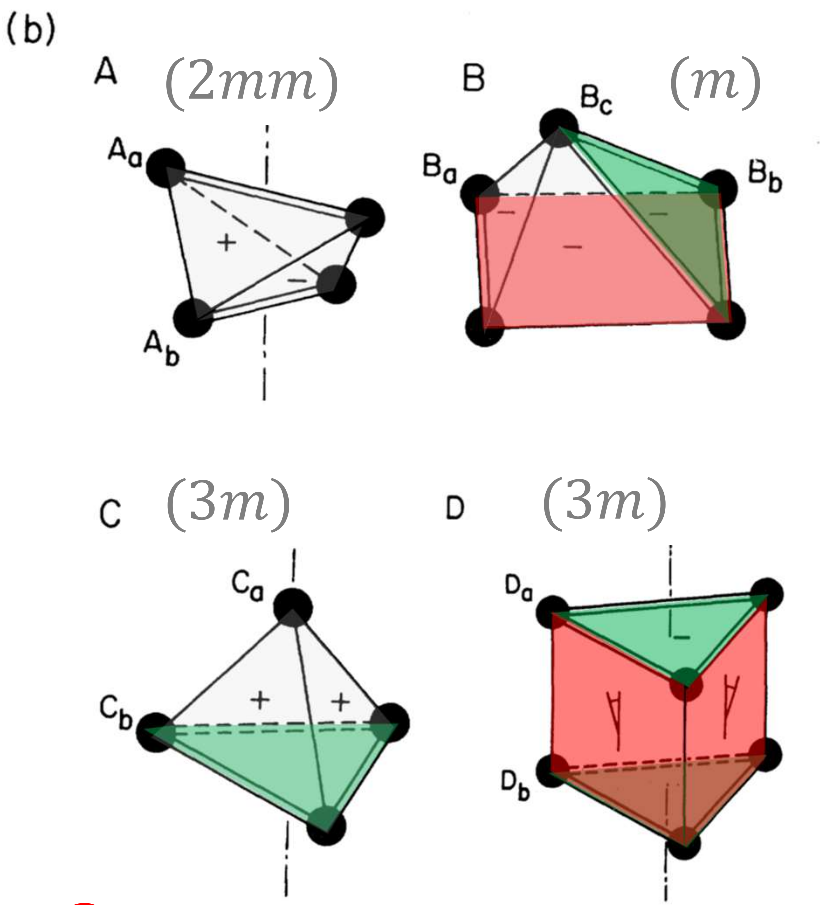
Large approximants in Al-based alloys

Atomic decoration model of CCT

Microscopic twinning

§ Geometrical basis of CCT

(for F-type structures)



8 4 kinds of cell (3D)

2 1 kind of node ($\bar{5}\bar{3}2/m$)

Parity + / −

3 2 kinds of edge

b-linkages (// 2-fold, mmm)

c-linkages (// 3-fold, $\bar{3}m$)

$b : c = 2 : \sqrt{3}$

5 3 kinds of face

X-face (isosceles tr., m)

Y-face (equilateral tr., $3m$)

Z-face (rectangle, $2/m$)

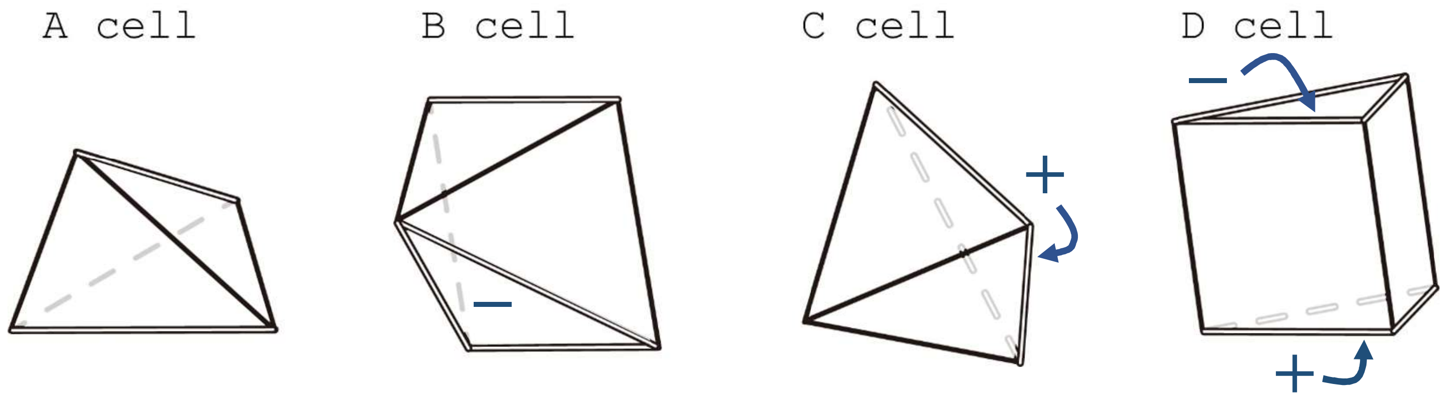
Cell geometry for cluster-based quasicrystal models
C. L. Henley, *Phys. Rev. B* 43, 993 (1991).

2019),

Face matching constraints

X face → shared by AB, AC, or BC pairs

Y face → shared by BC, BD, or CD pairs

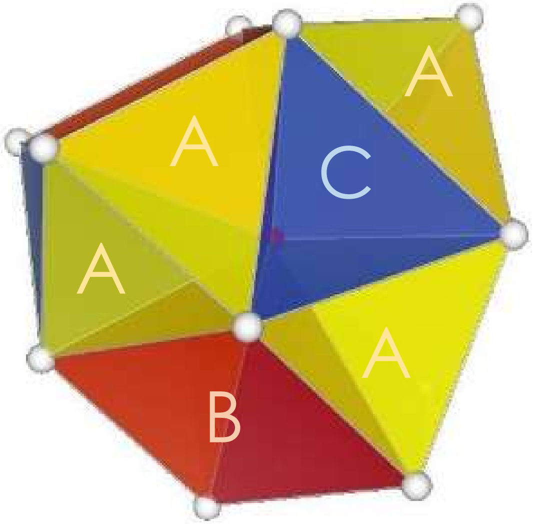


charge neutrality ⟹ Equal number of B and C

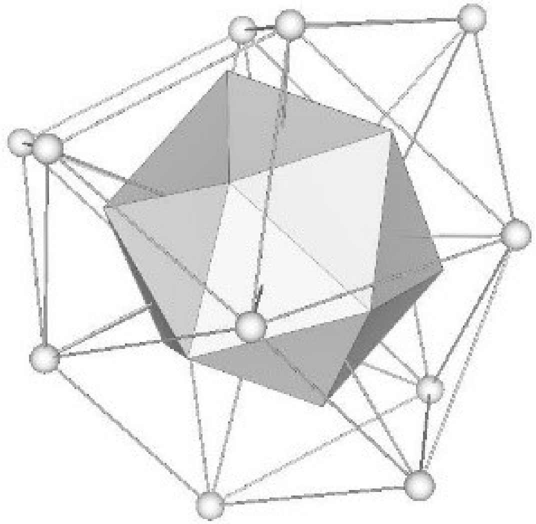
Z face → shared by BB, BD, or DD pairs

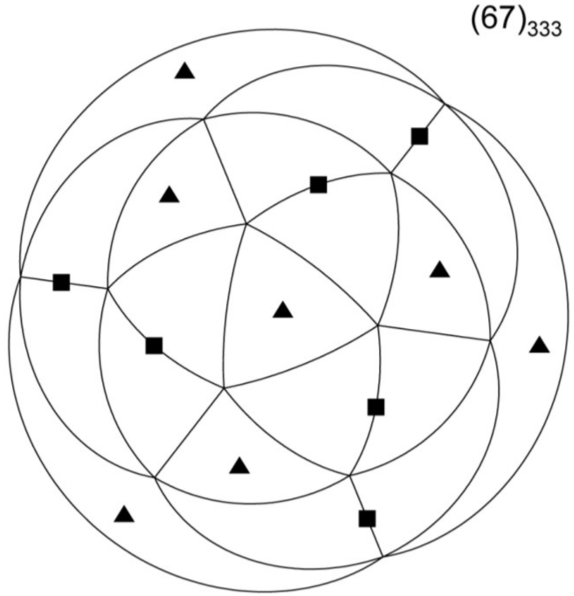
Allowed node environments

$(67)_{333}$

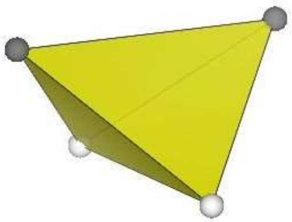


3

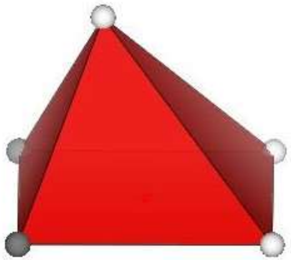




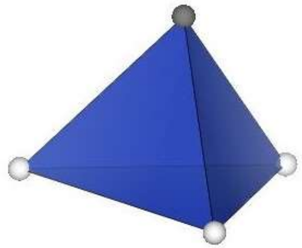
A



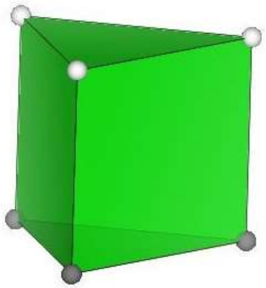
B



C

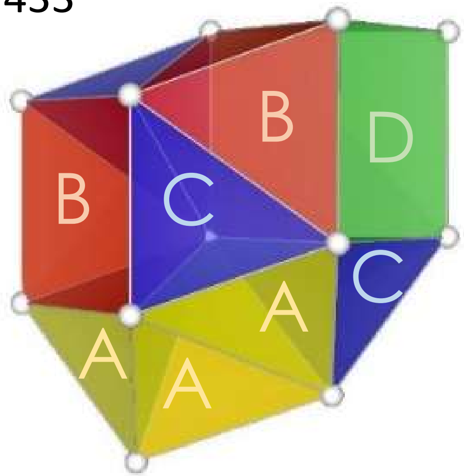


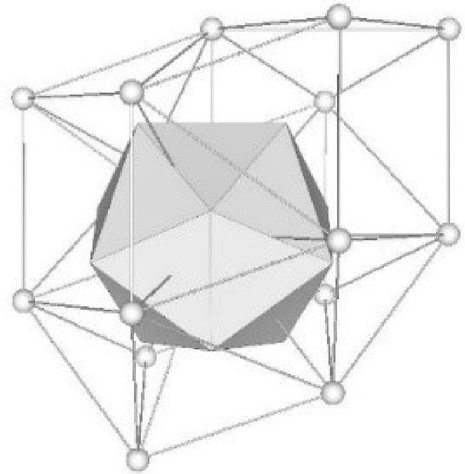
D

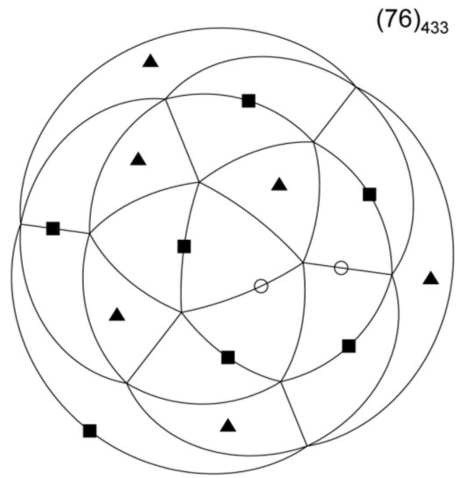


Allowed node environments

$(76)_{433}$

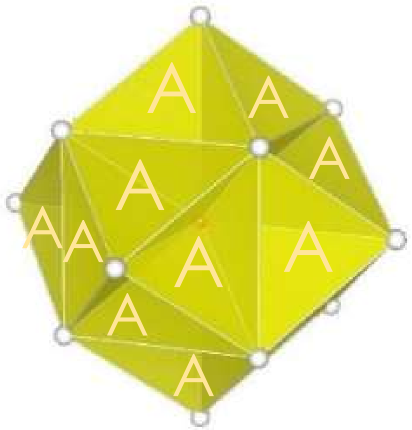


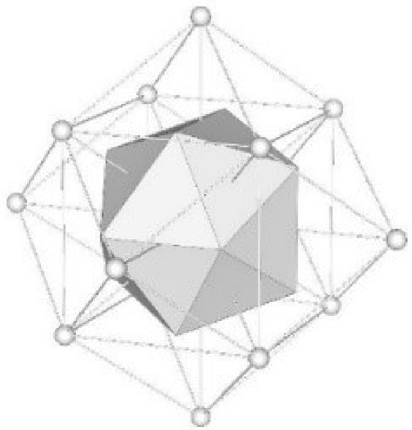


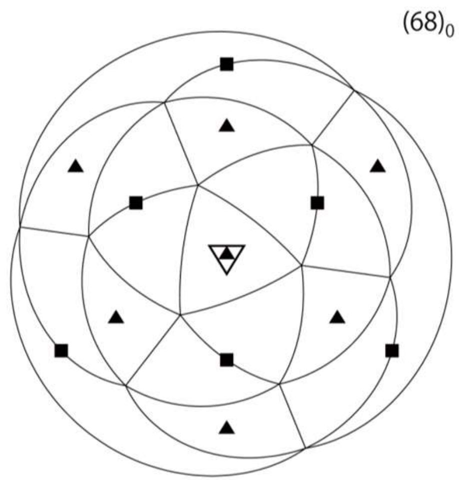


1

$(68)_0$

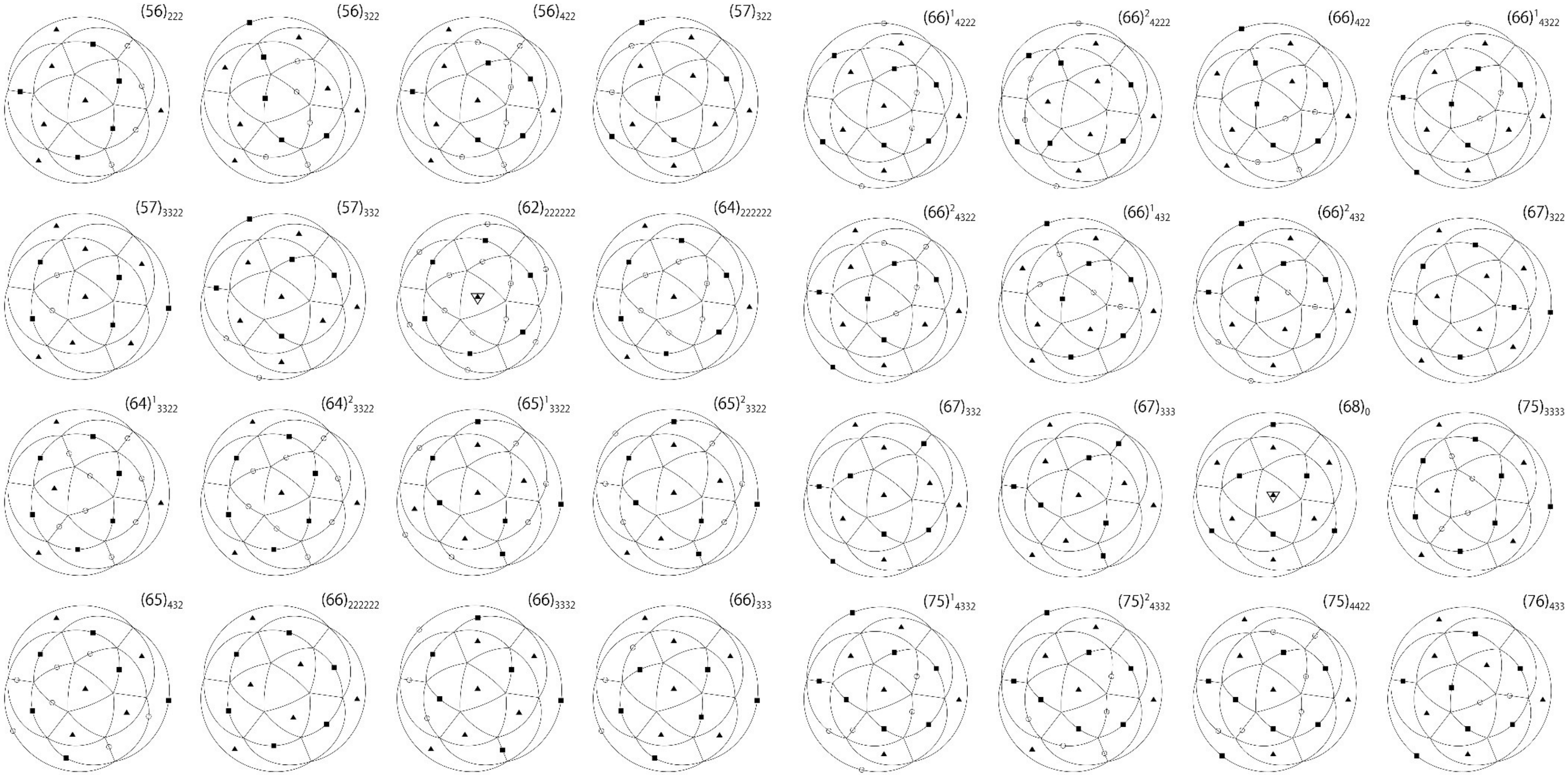






$m\bar{3}$

Allowed node environments (32)

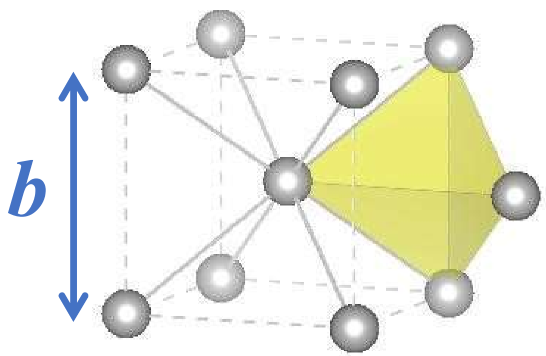


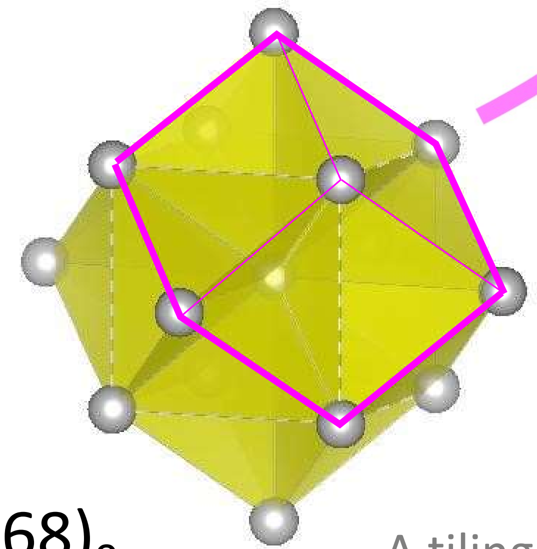
C. L. Henley, *Phys. Rev. B* 43, 993 (1991).
(Fig. taken from N. F., Annals of Physics **385** (2017) 225.)

19),

§ Simplest examples

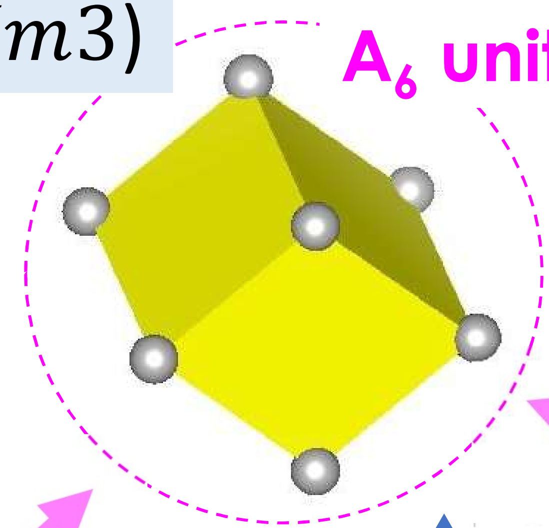
1/1 cubic (bcc, $Im\bar{3}$)

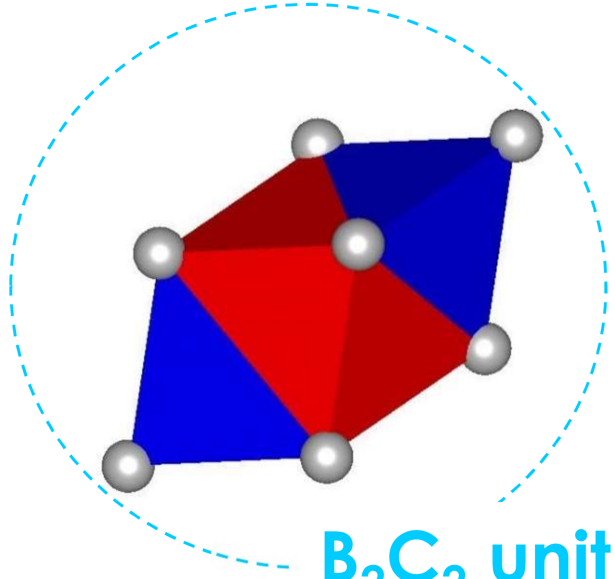


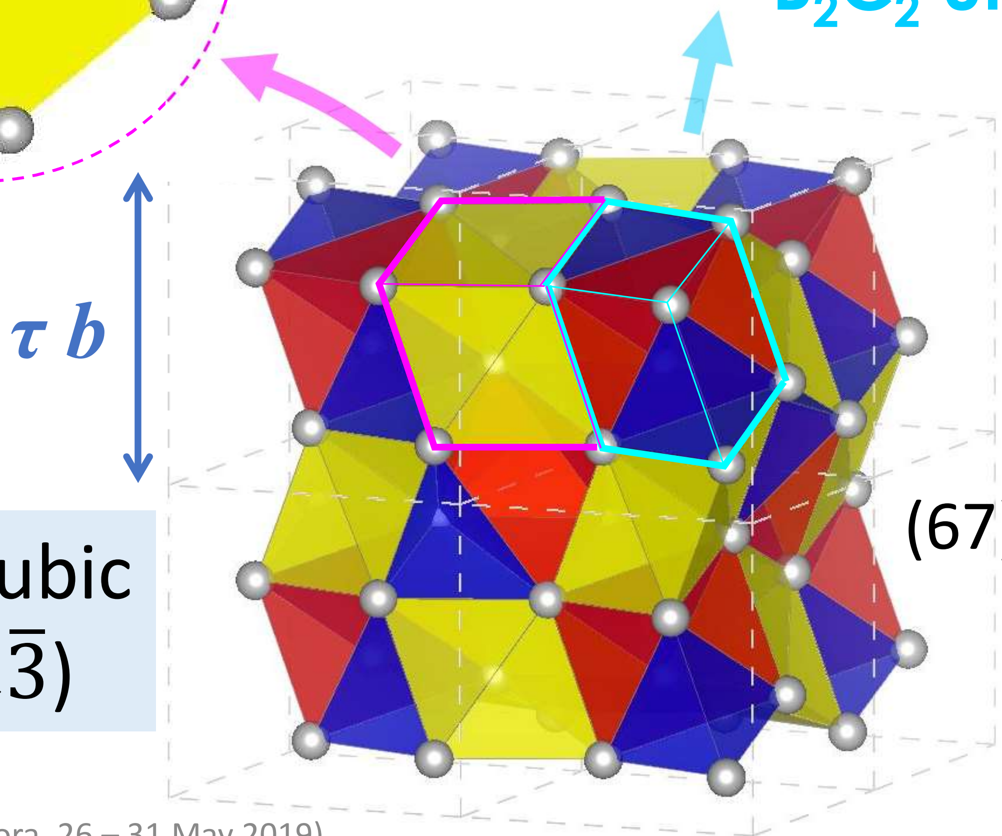


$(68)_0$

A tiling





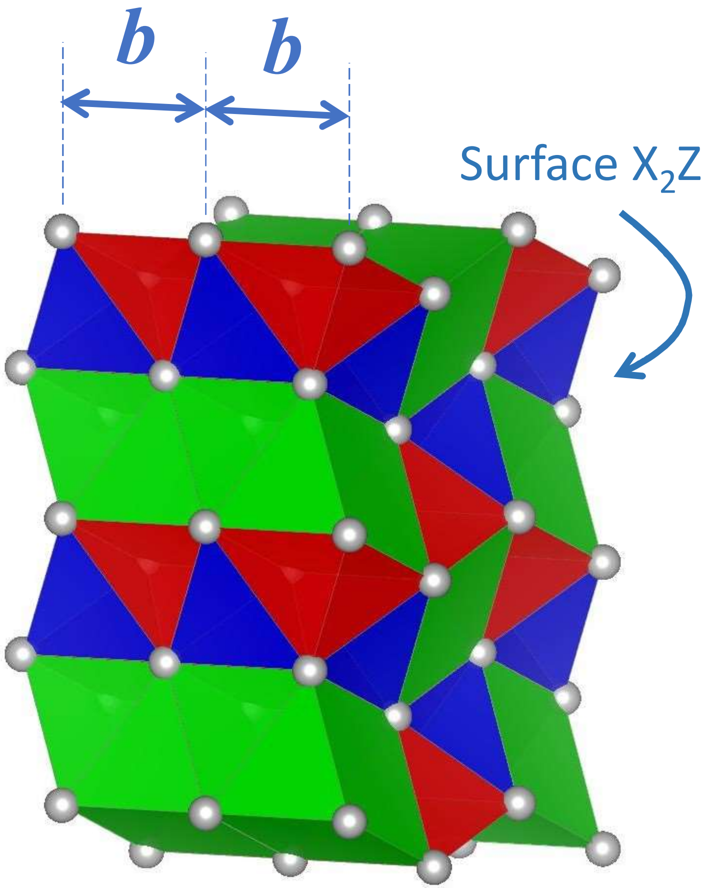


2/1 cubic ($Pa\bar{3}$)

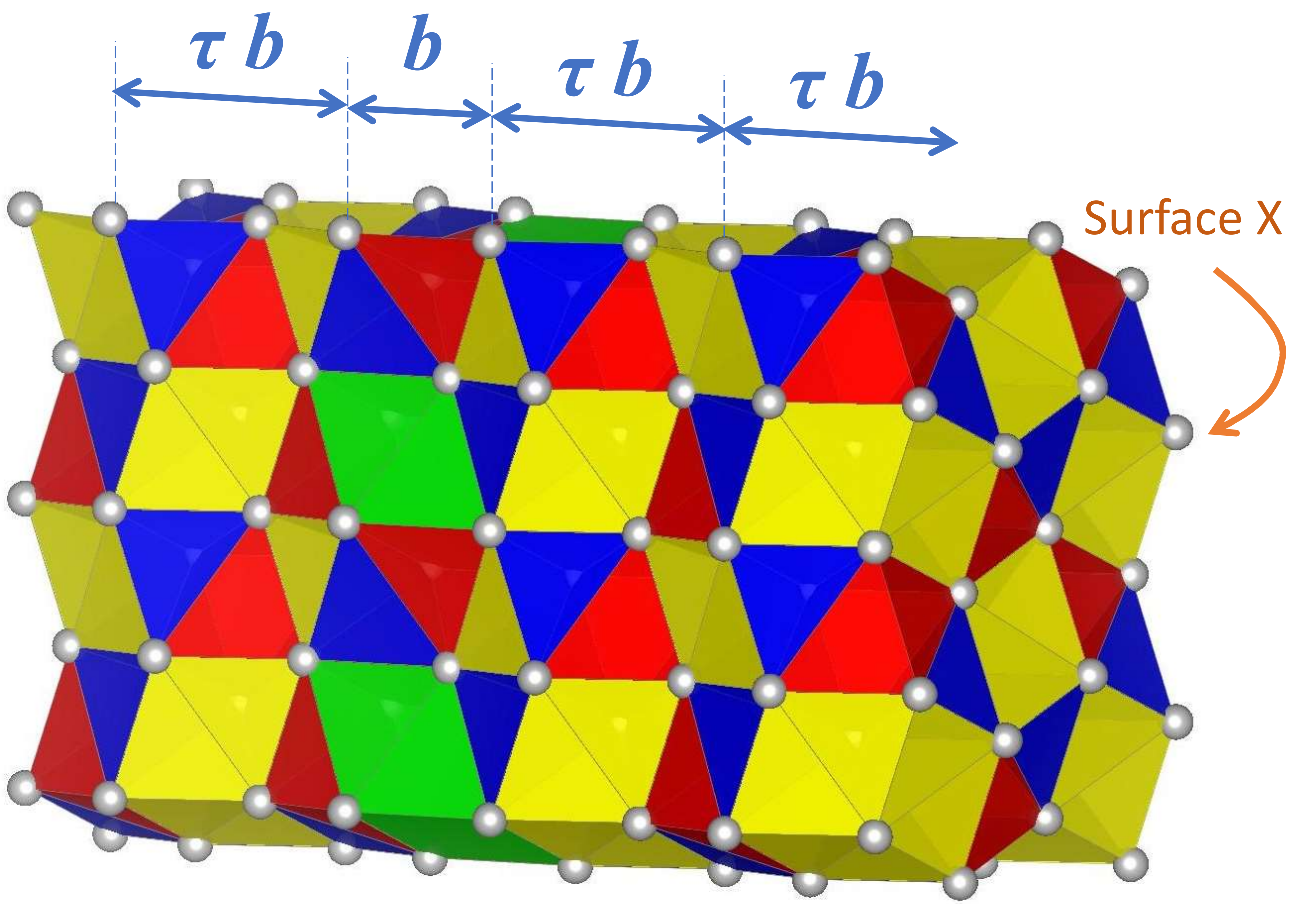
$(67)_{333}$

ABC tiling

More examples



BCD tiling

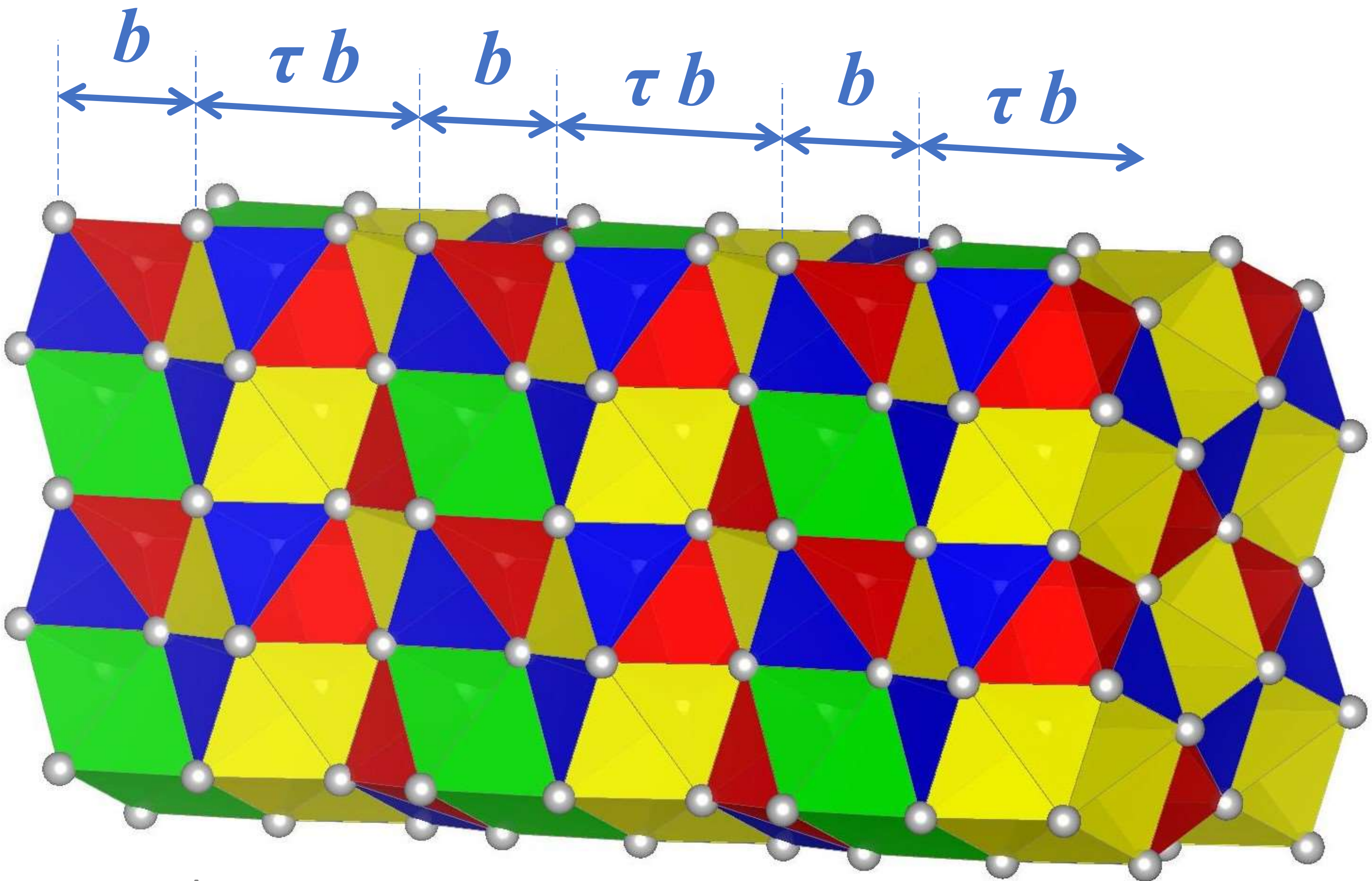


ABC(D) tiling

$(2/1)^2(1/1)$ orthorhombic ($Pnma$)

2/1 cubic + stacking fault ($Pa\bar{3}$)

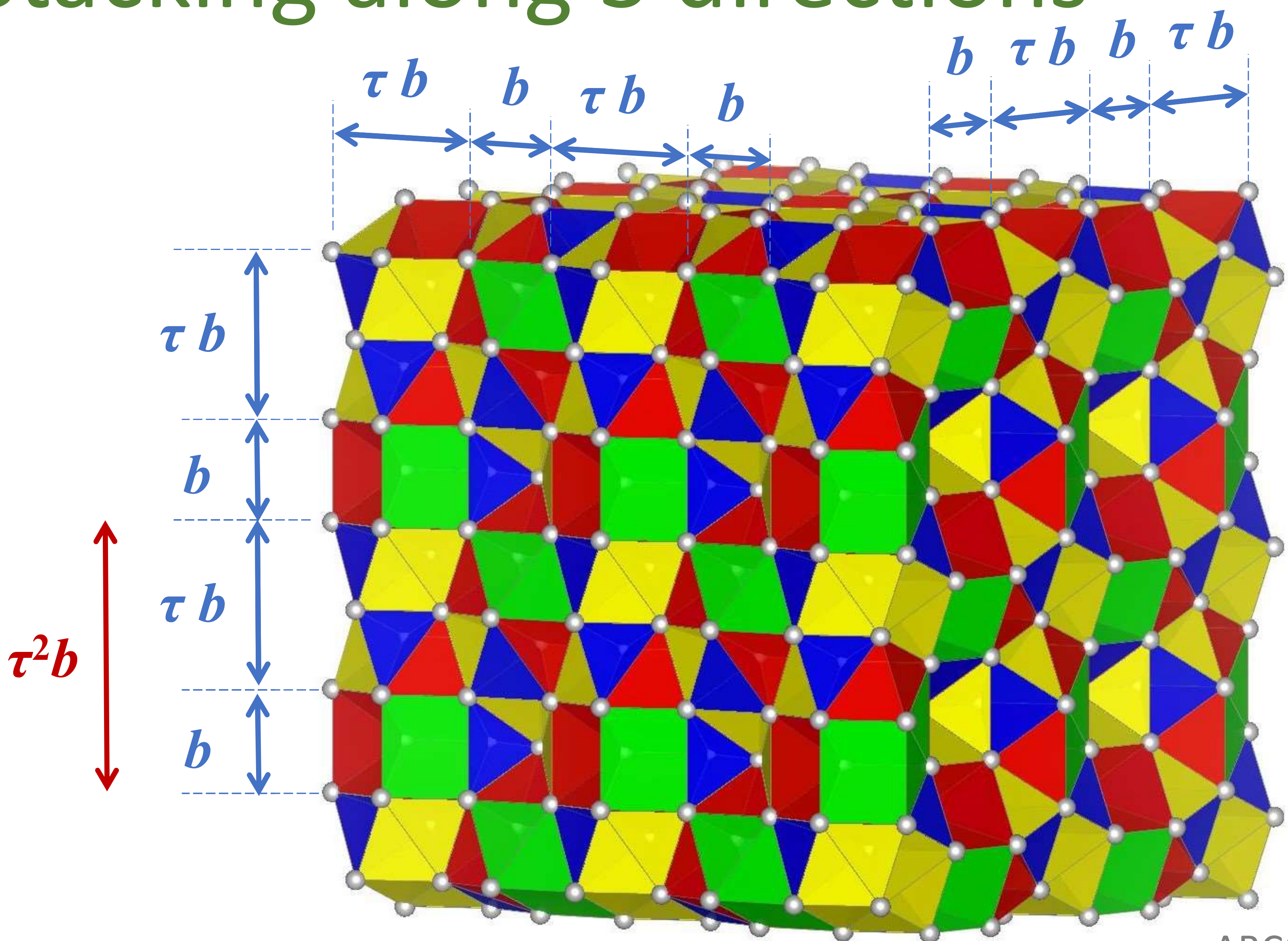
Layered stacking (→Fibonacci CCT)



ABCD tiling

(2/1)²(3/2) monoclinic ($P2_1/c$)

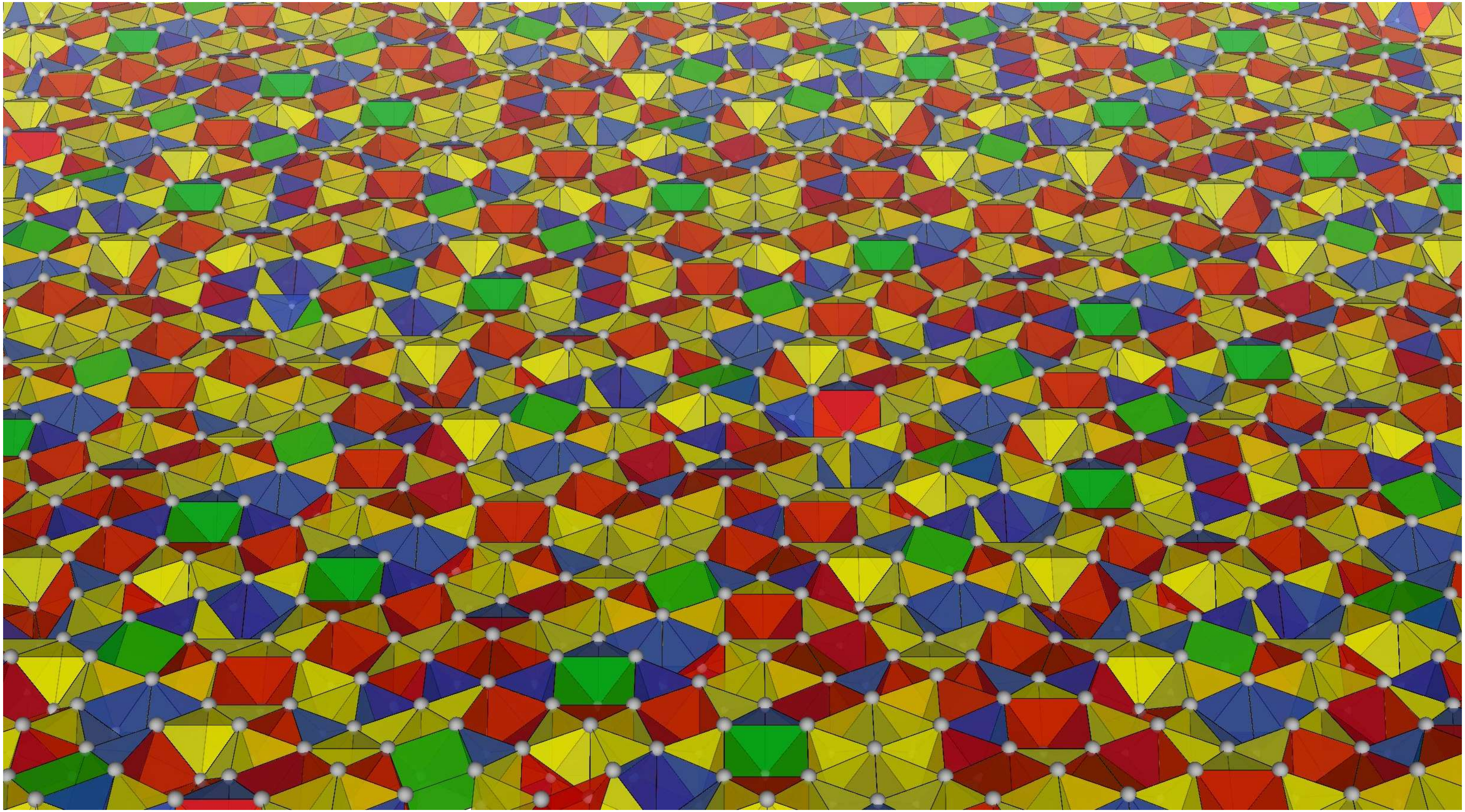
Stacking along 3 directions



ABC(D) tiling

(3/2)³ rhombohedral ($R\overline{3}$) … a variant of 3/2 cubic

§ Quasiperiodic CCT



N. F., Annals of Physics **385** (2017) 225—286.

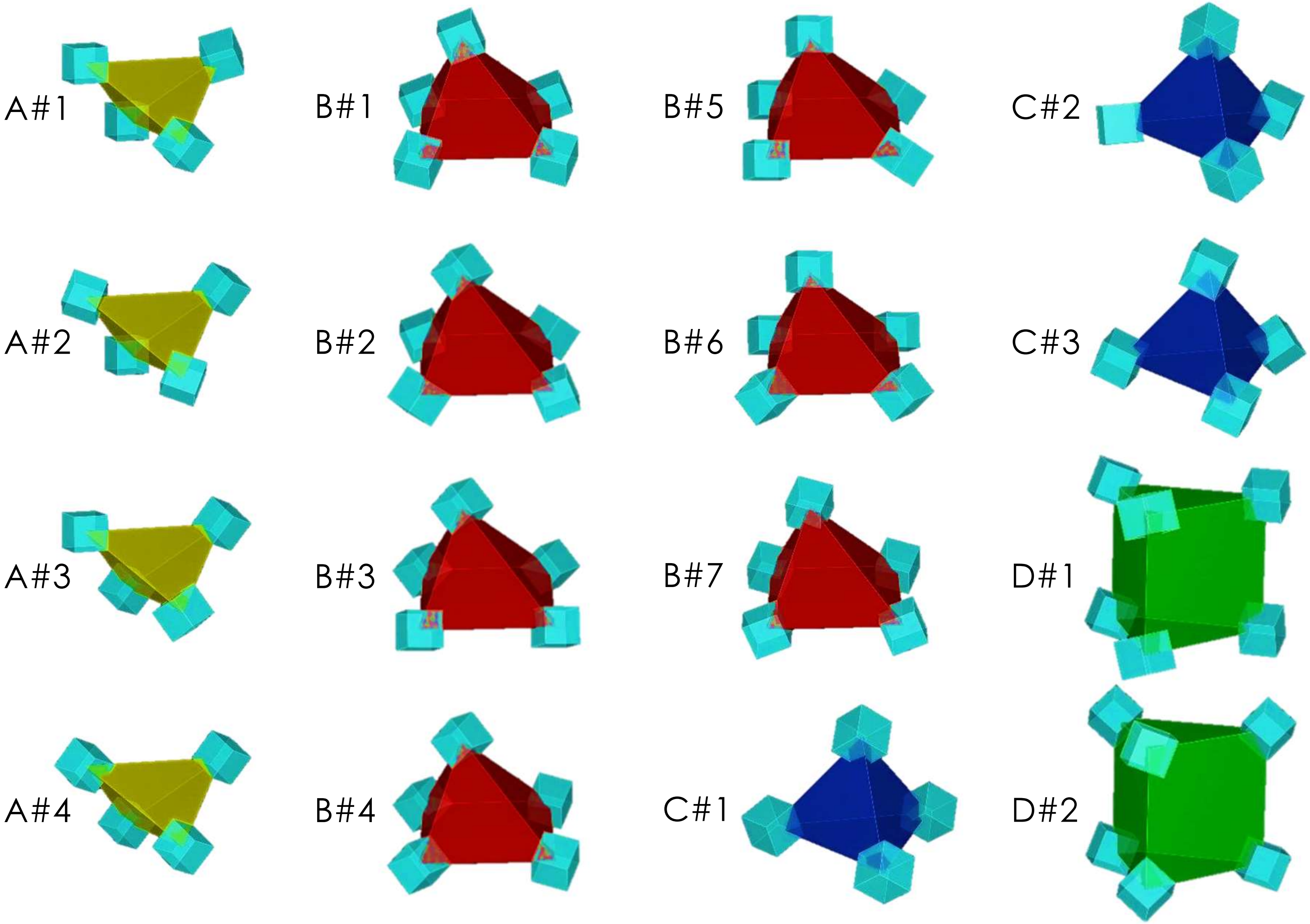
16 cells with symmetry restraints

Symmetry of node

$\bar{5}\bar{3}2/m$

↓

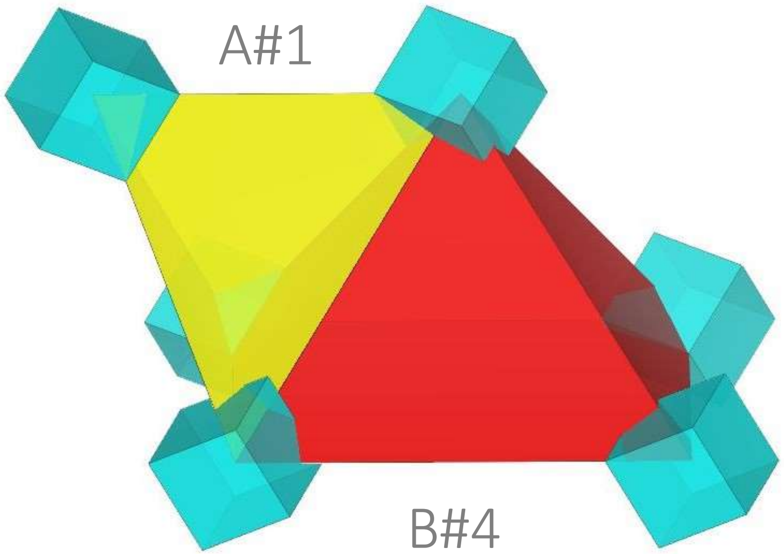
$m\bar{3}$



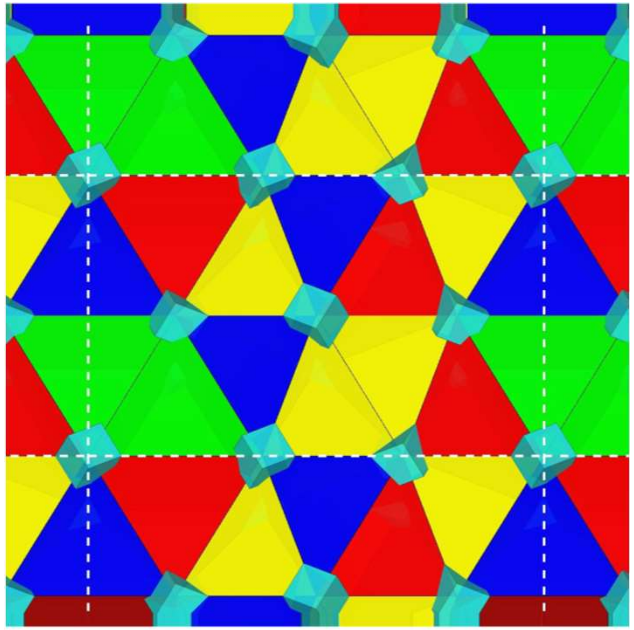
N. F., Annals of Physics **385** (2017) 225—286.

Matching constraints

Blue cubes attached to the nodes constrain the matching of cells



A periodic example satisfying the matching constraints

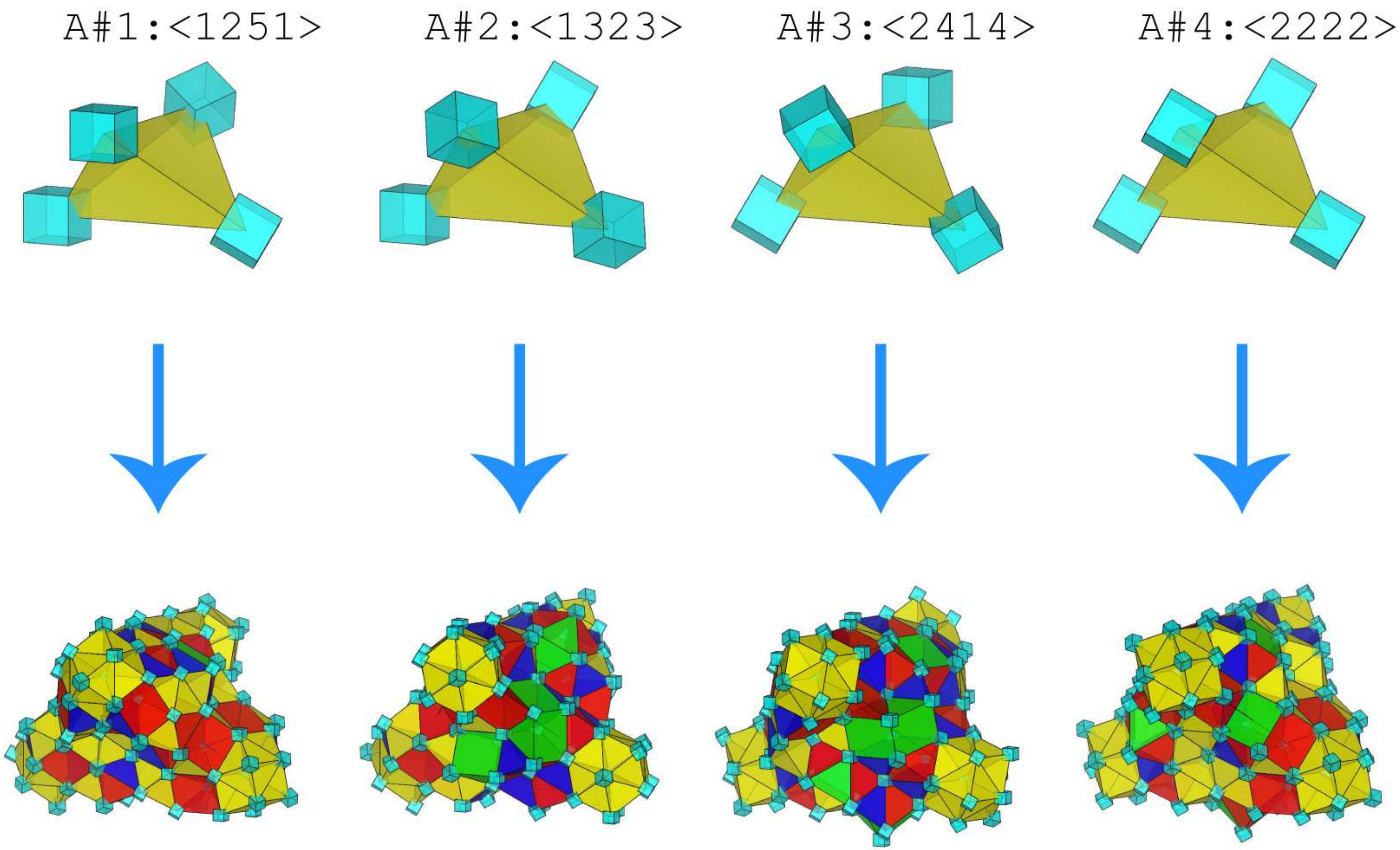


A#1 x 24
B#2 x 8
B#4 x 4
C#2 x 8
C#3 x 4
D#2 x 4

$(2/1)^2$ 3/2 monoclinic packing ($P2_1/c$)

N. F., Annals of Physics **385** (2017) 225—286.

τ^3 inflation: subdivision of cells

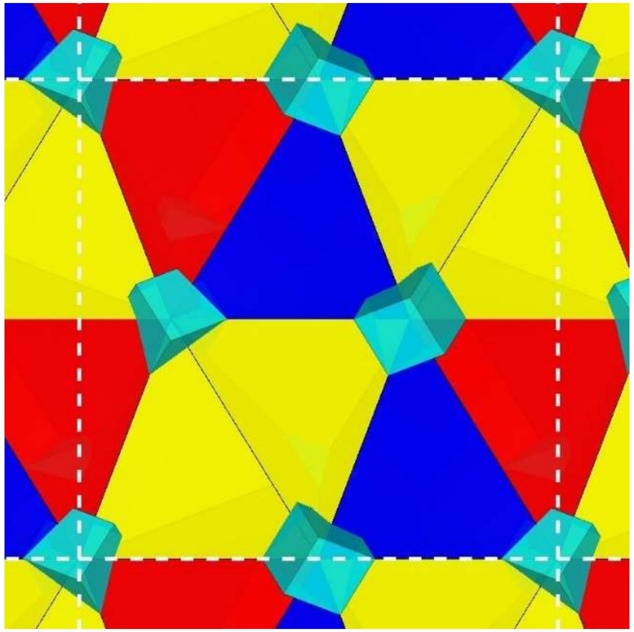


Unique subdivision rules identified for the 16 cells

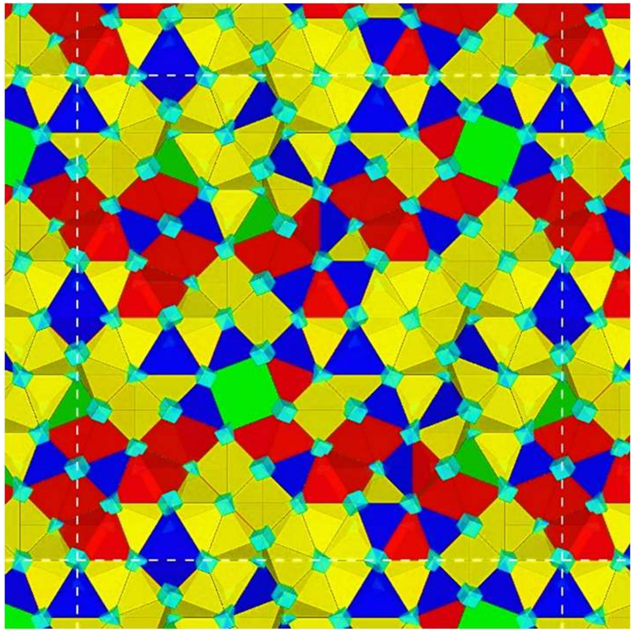
N. F., Annals of Physics **385** (2017) 225—286.

An iteration of the τ^3 inflation

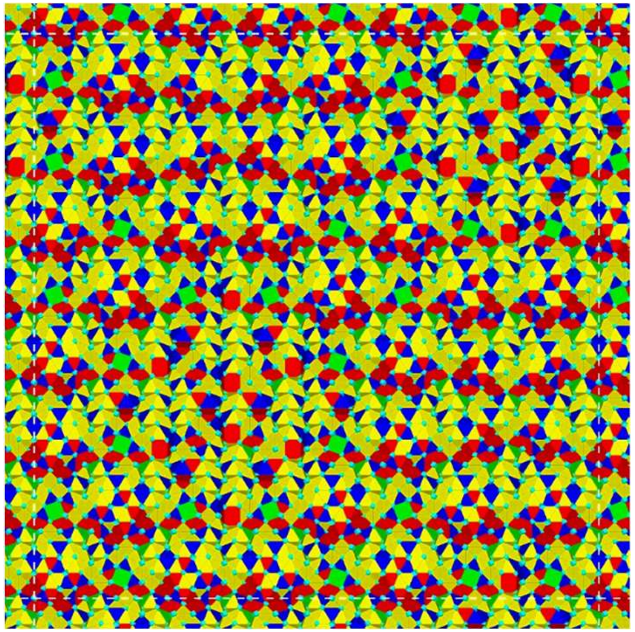
2/1 cubic packing
$(Pa\bar{3})$



8/5 cubic packing
$(Pa\bar{3})$

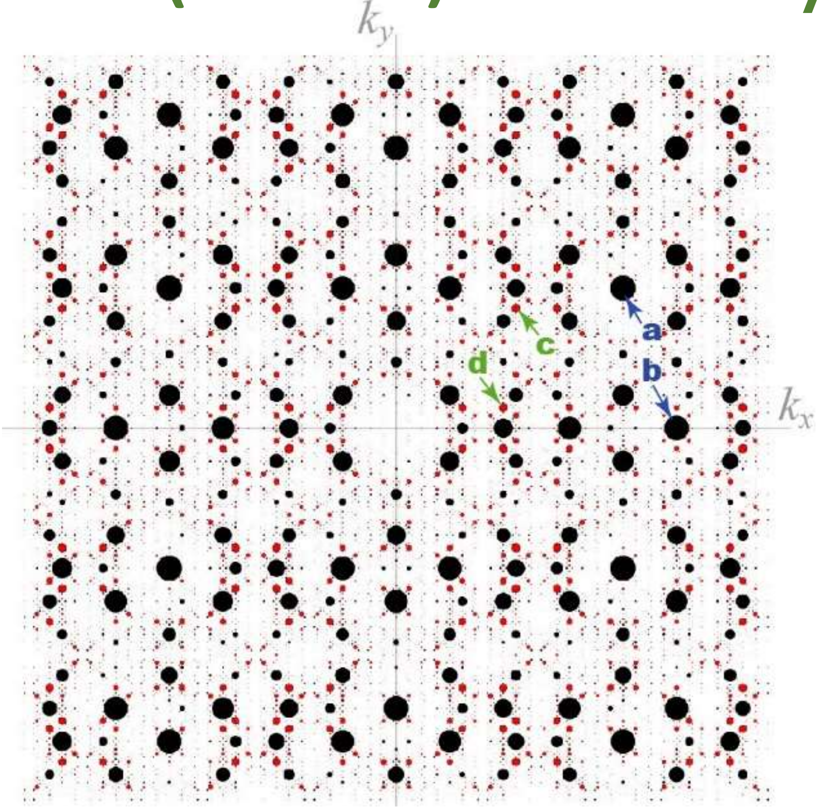


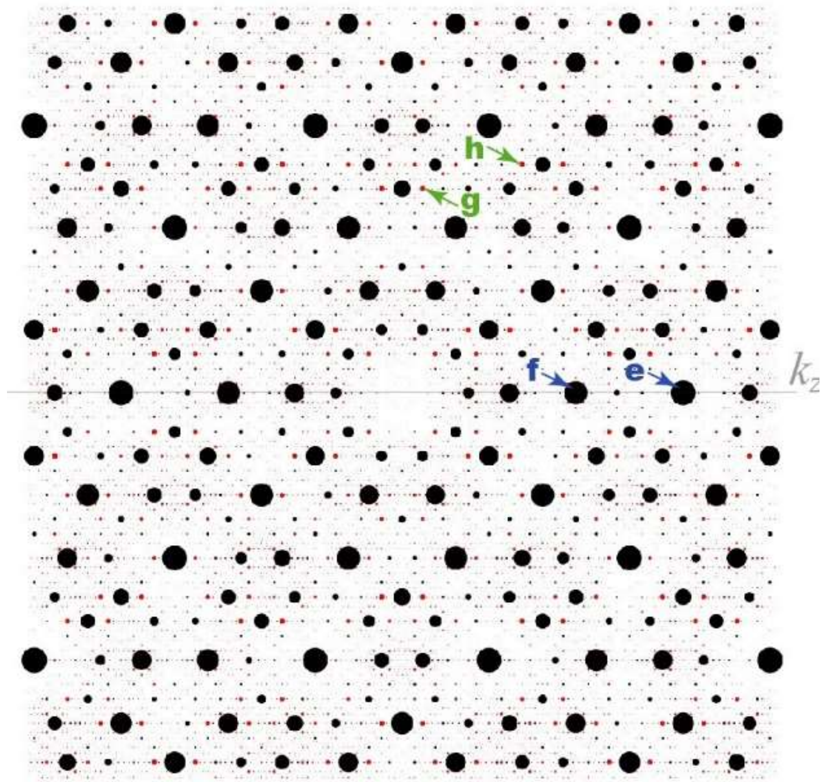
34/21 cubic packing
$(Pa\bar{3})$



N. F., Annals of Physics **385** (2017) 225—286.

Point symmetry breaking : $m\bar{3}$ (tetra) $\subset$ $\bar{5}\bar{3}2/m$ (icosa)





Almost icosahedral symmetry ($m\bar{3}$ modulation)

N. F., Annals of Physics **385** (2017) 225—286.

Application of CCT

§ Large approximant structures

§ Atomic decoration model

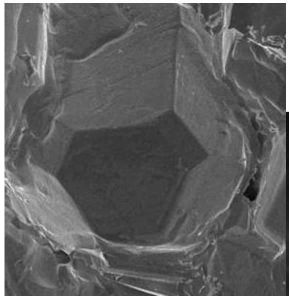
§ Microscopic twinning

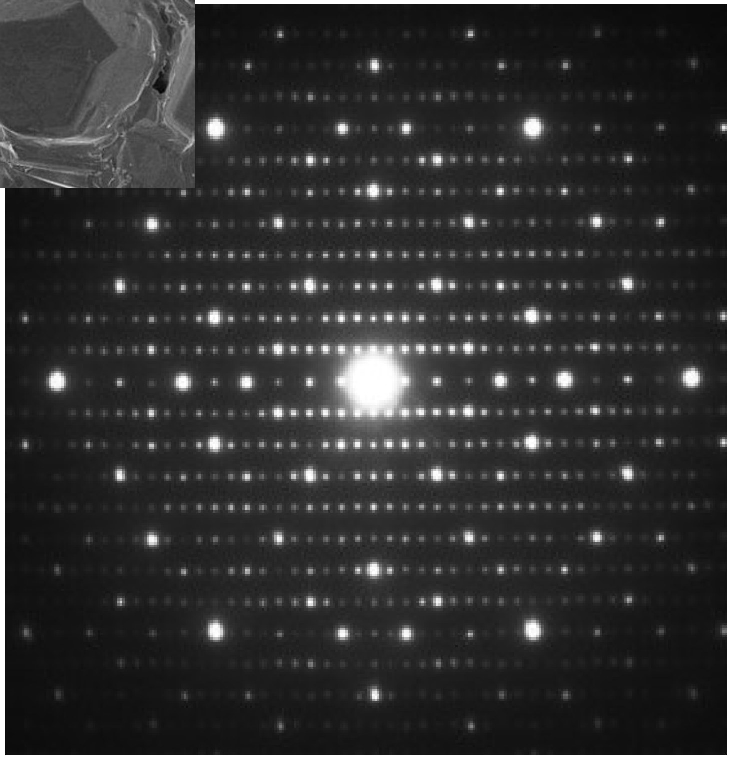
§ Large approximant structures

Ø 0.3mm

$Al_{69}Pd_{22}Cr_2Fe_6$

$Pa\bar{3}\ \ a \cong 40.5\text{Å}$

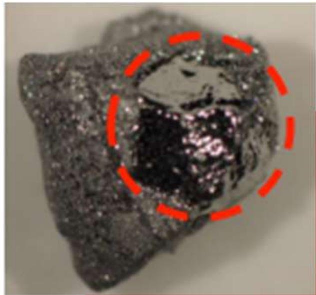


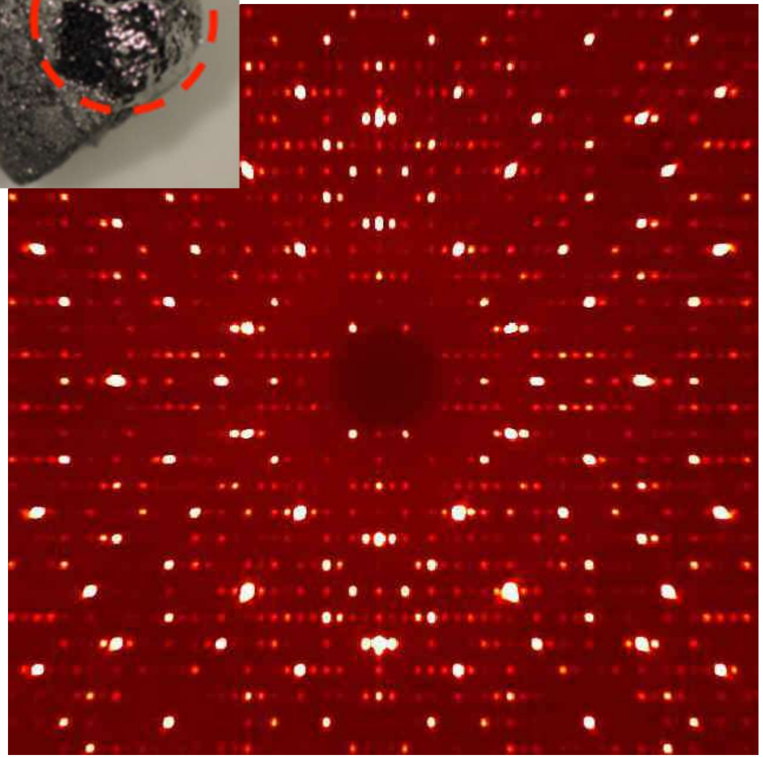


Ø 3mm

$Al_{72}Pd_{16}Ru_{12}$ (P_{40}-phase)

$Pa\bar{3}\ \ a \cong 40.7\text{Å}$



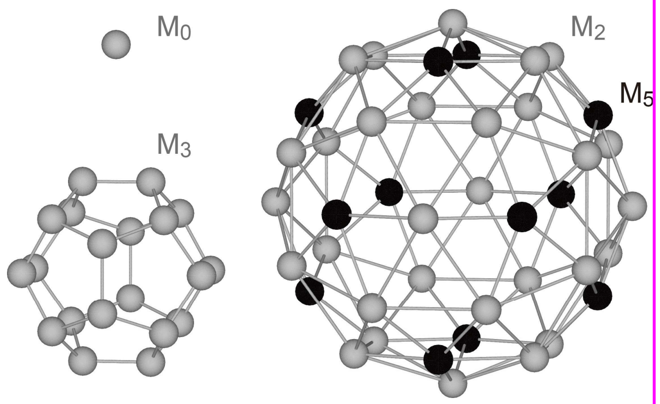


N. F., *et al.*
Acta Cryst. A **69**, 322 (2013)

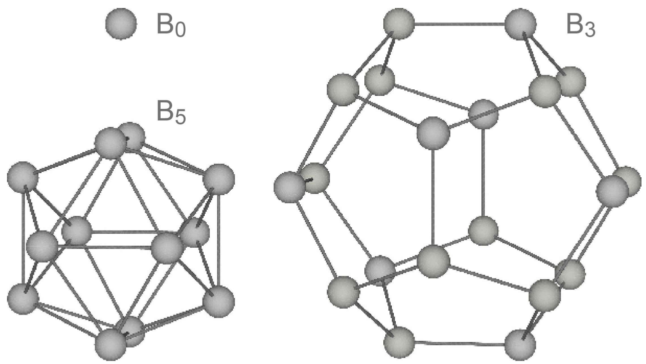
Y. Hatakeyama, *et al.*
J. Phys: Conf. Ser. **809** (2017) 012007.

(2x2x2) 3/2 cubic approximant

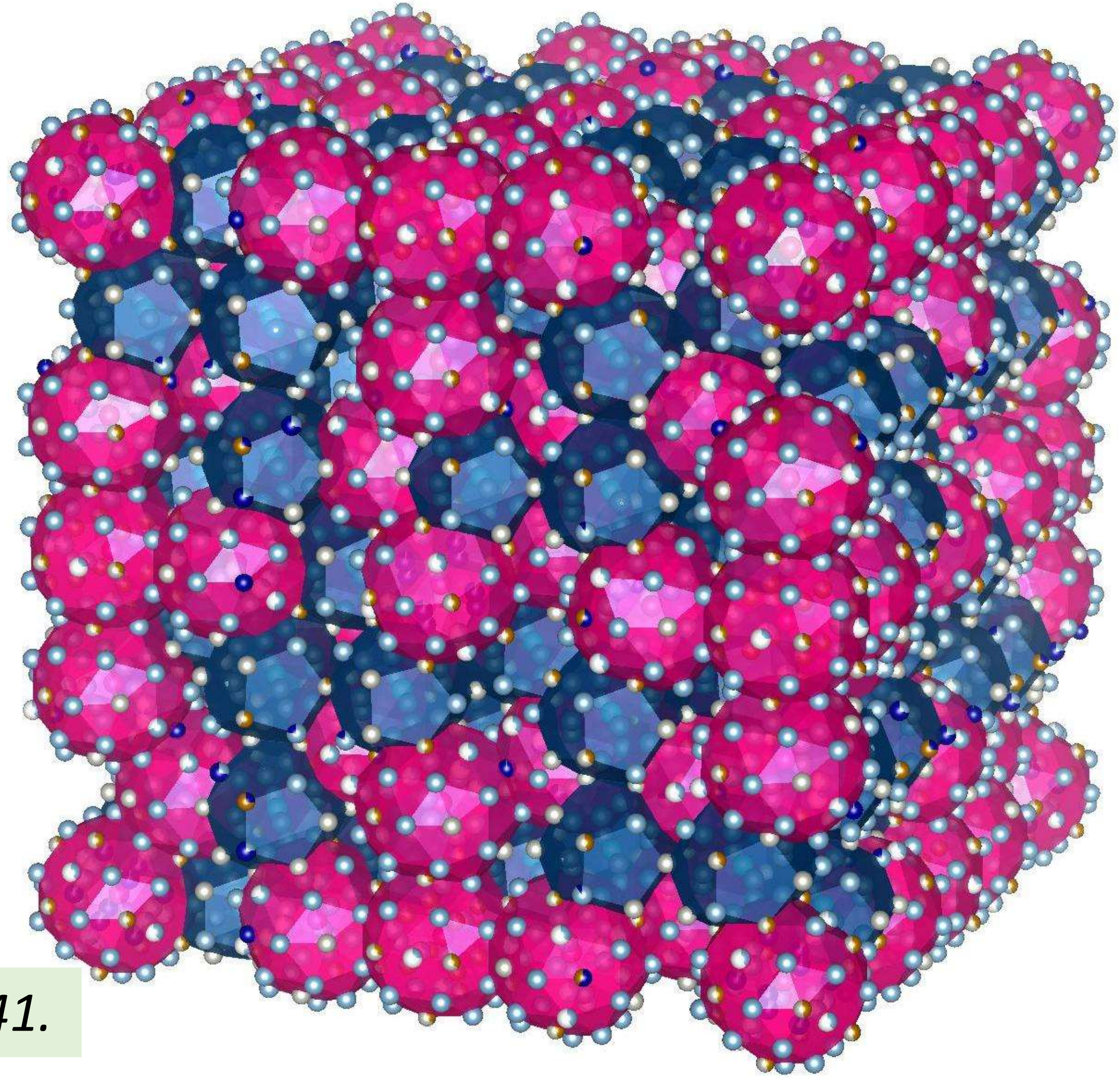
$a = 40.54\text{Å}, Pa\overline{3}$



pseudo-Mackay cluster



mini-Bergman cluster



Cf. V. Elser, Phil. Mag. B ***73*** *(1996) 641.*

$Al_{69}Pd_{22}Cr_2Fe_6$

N. F. *et al.*, Acta Cryst. A **69**, 322 (2013)

CCT for (2x2x2) 3/2 cubic AP

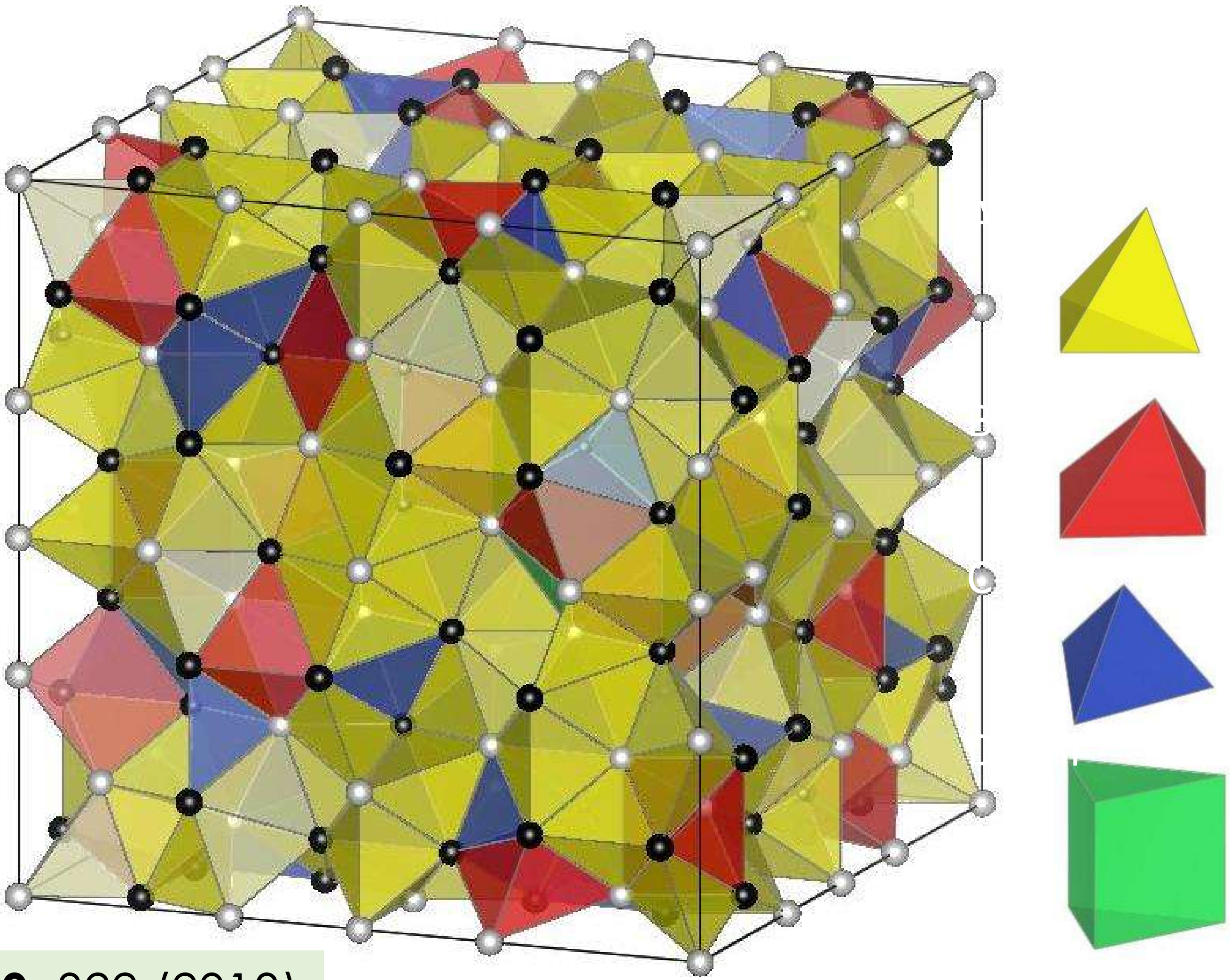
EVEN & ODD parities of nodes are distinguished

○

pseudo Makay cluster
centered at EVEN nodes

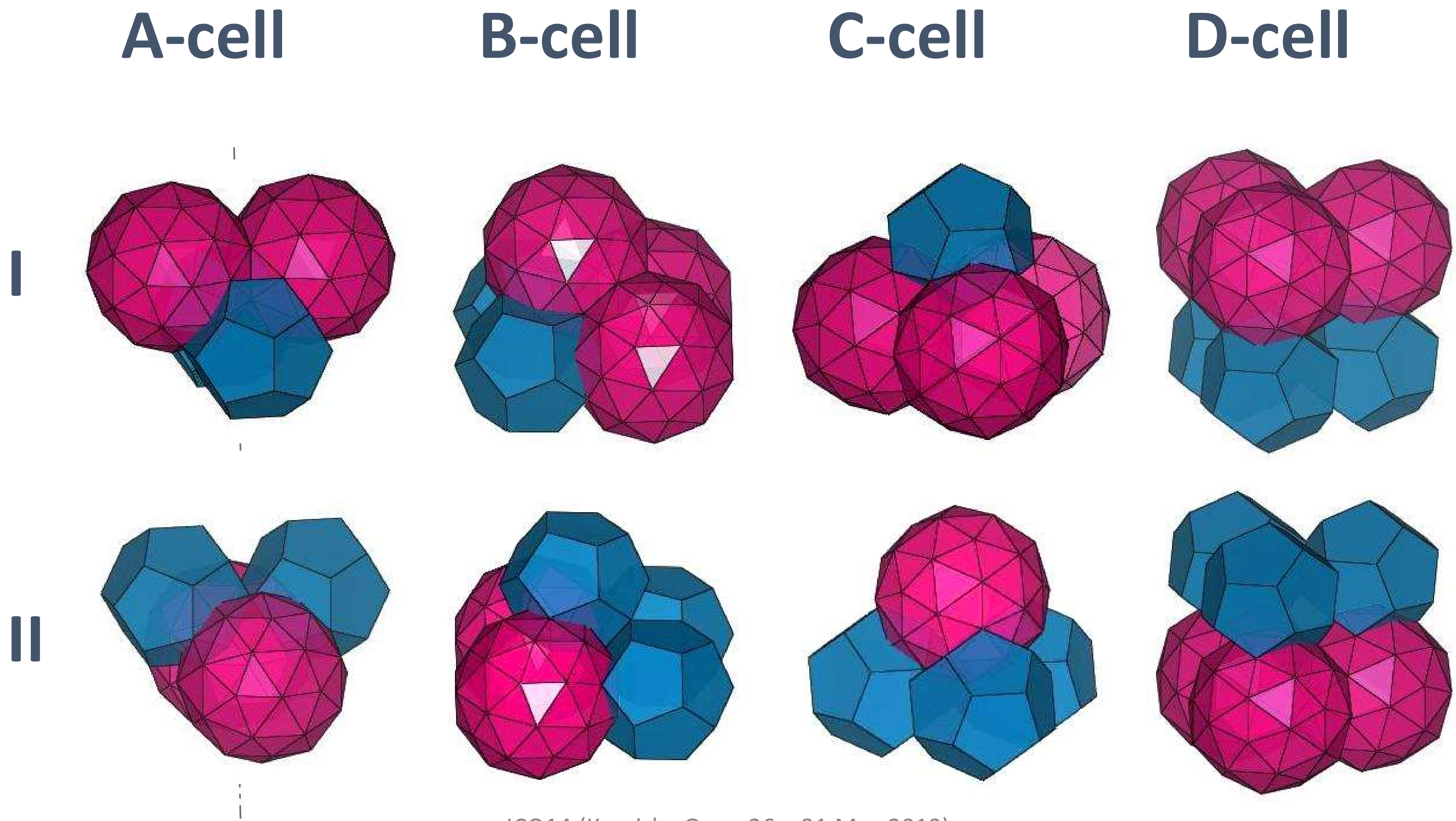
●

mini Bergman cluster
centered at ODD nodes



N. F. *et al.*, Acta Cryst. A **69**, 322 (2013)

Cell decorations with pMC & mBC

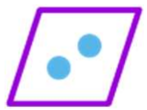


§ Atomic decoration model

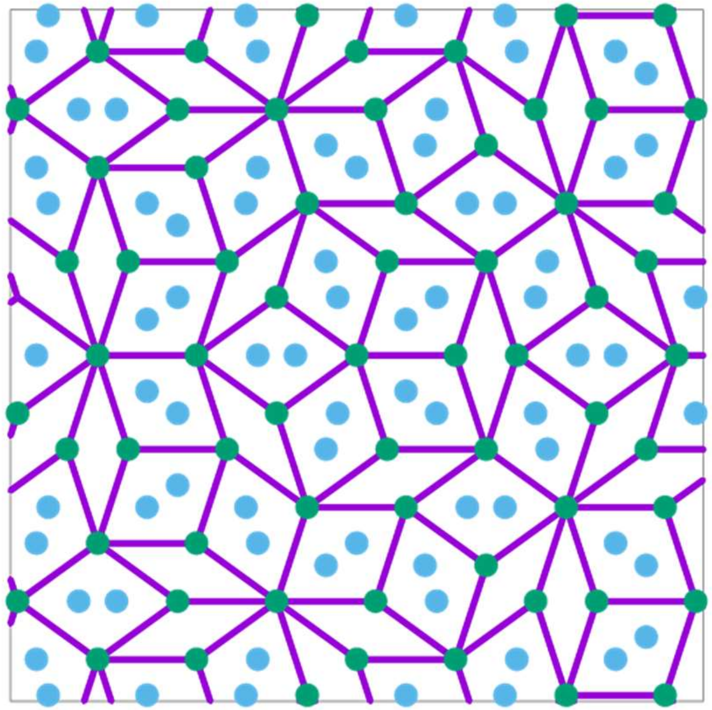
"Decoration model" is defined if the atomic decoration sites associated with *tiling objects* (node, edge, face, cell, or any combination of them) are specified, such that all the atoms in the structure are covered without any redundancy (overlap).

(Decoration sites)

Node (10mm)

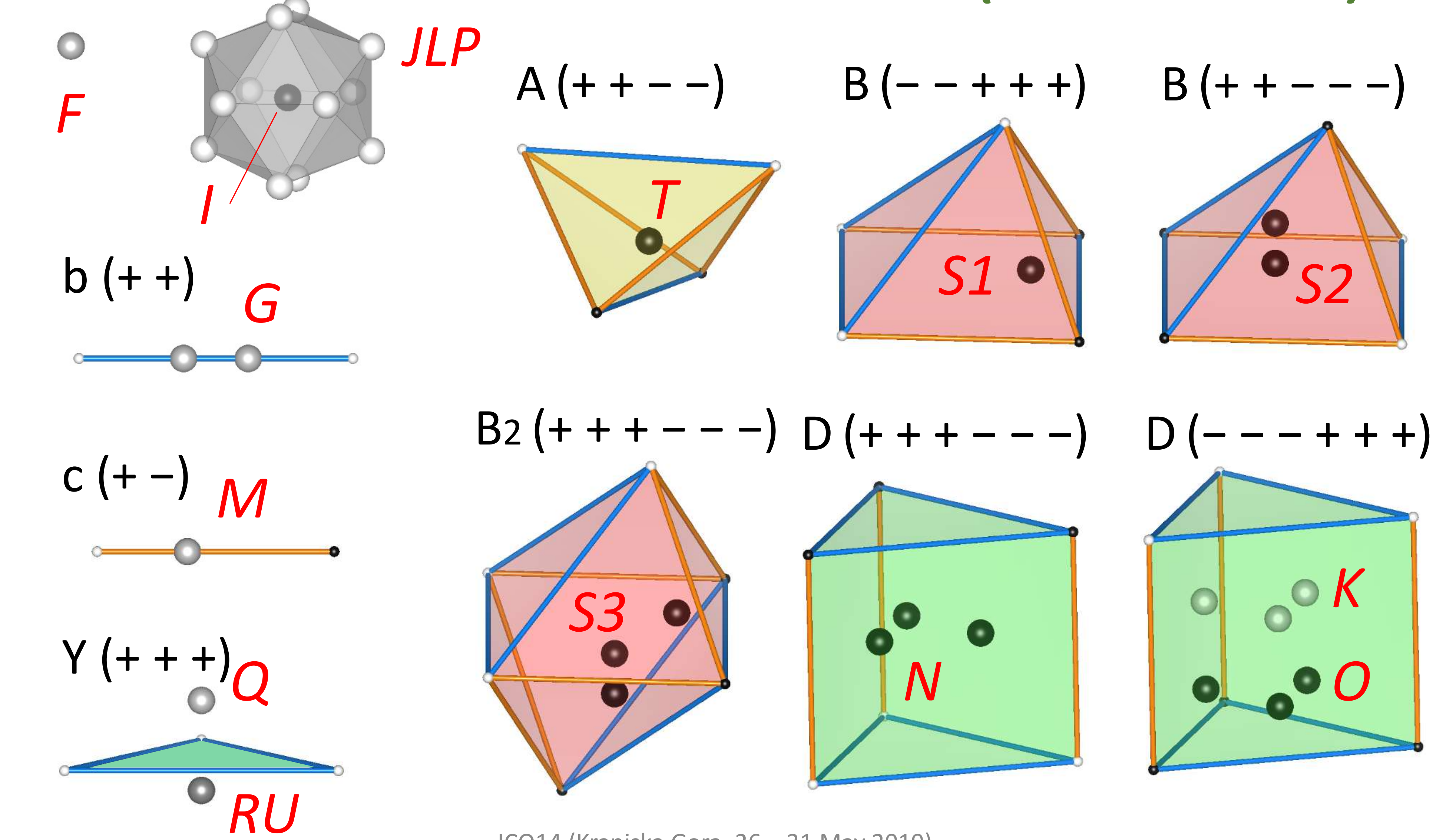


Fat rhombus (2mm)

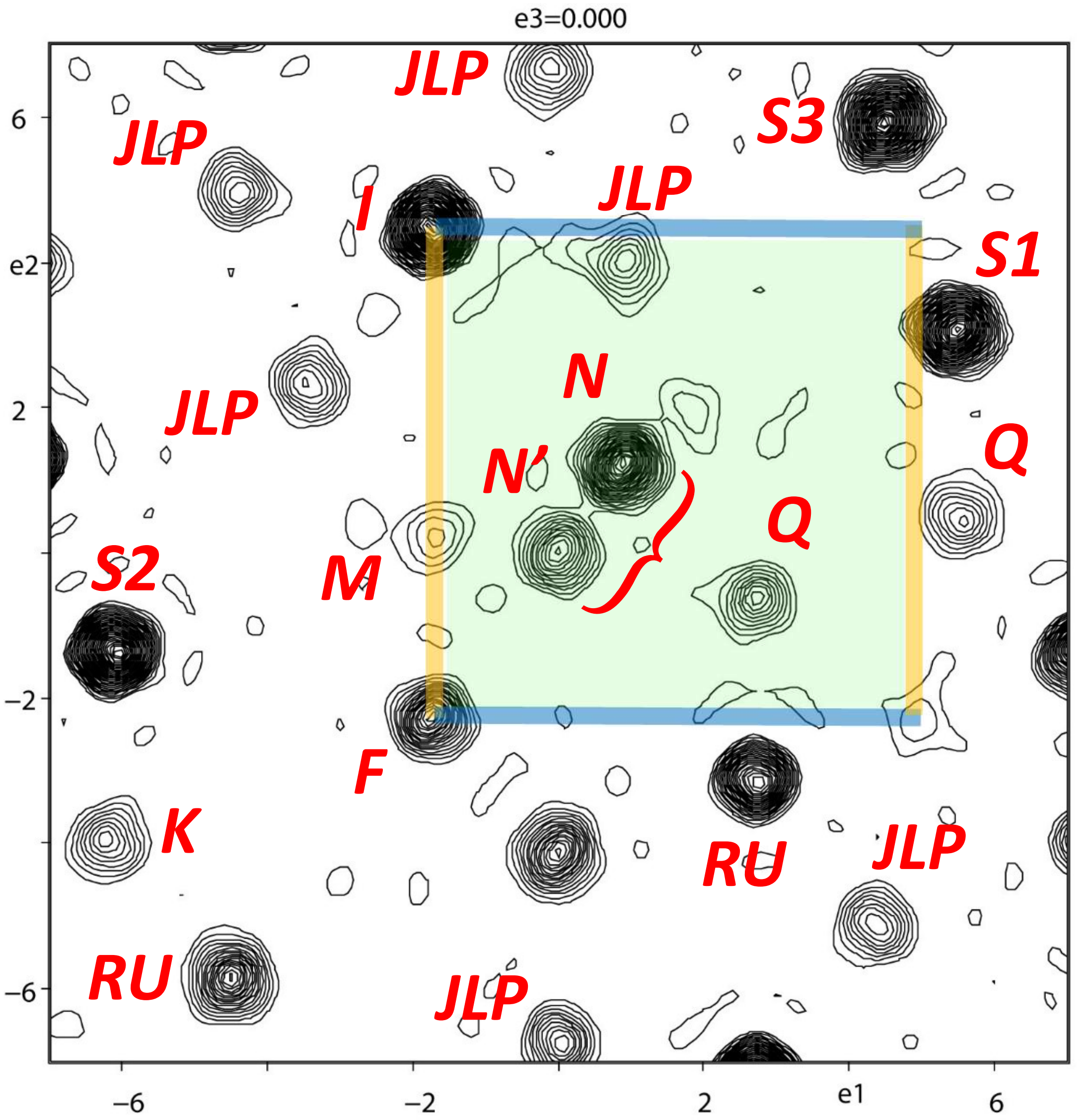


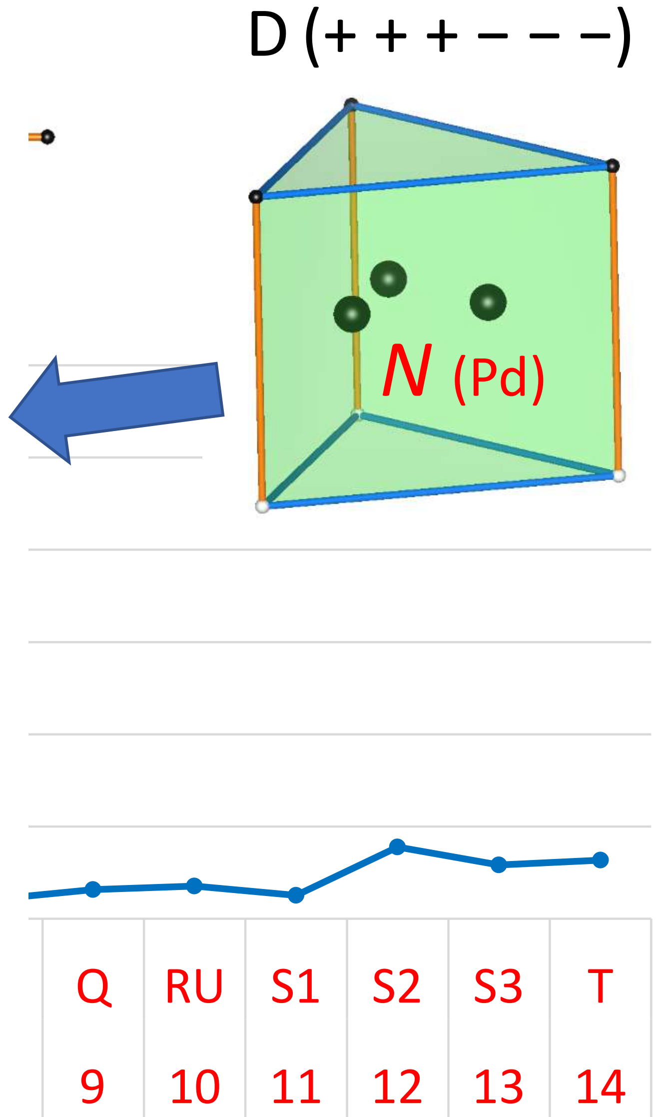
Icosahedral quasicrystal decoration models. I. Geometrical principles
M. Mihalkovič, *et al.*, *Phys. Rev. B* 43, 993 (1991).

Ideal decoration sites for Al-Pd-M (14 orbits)

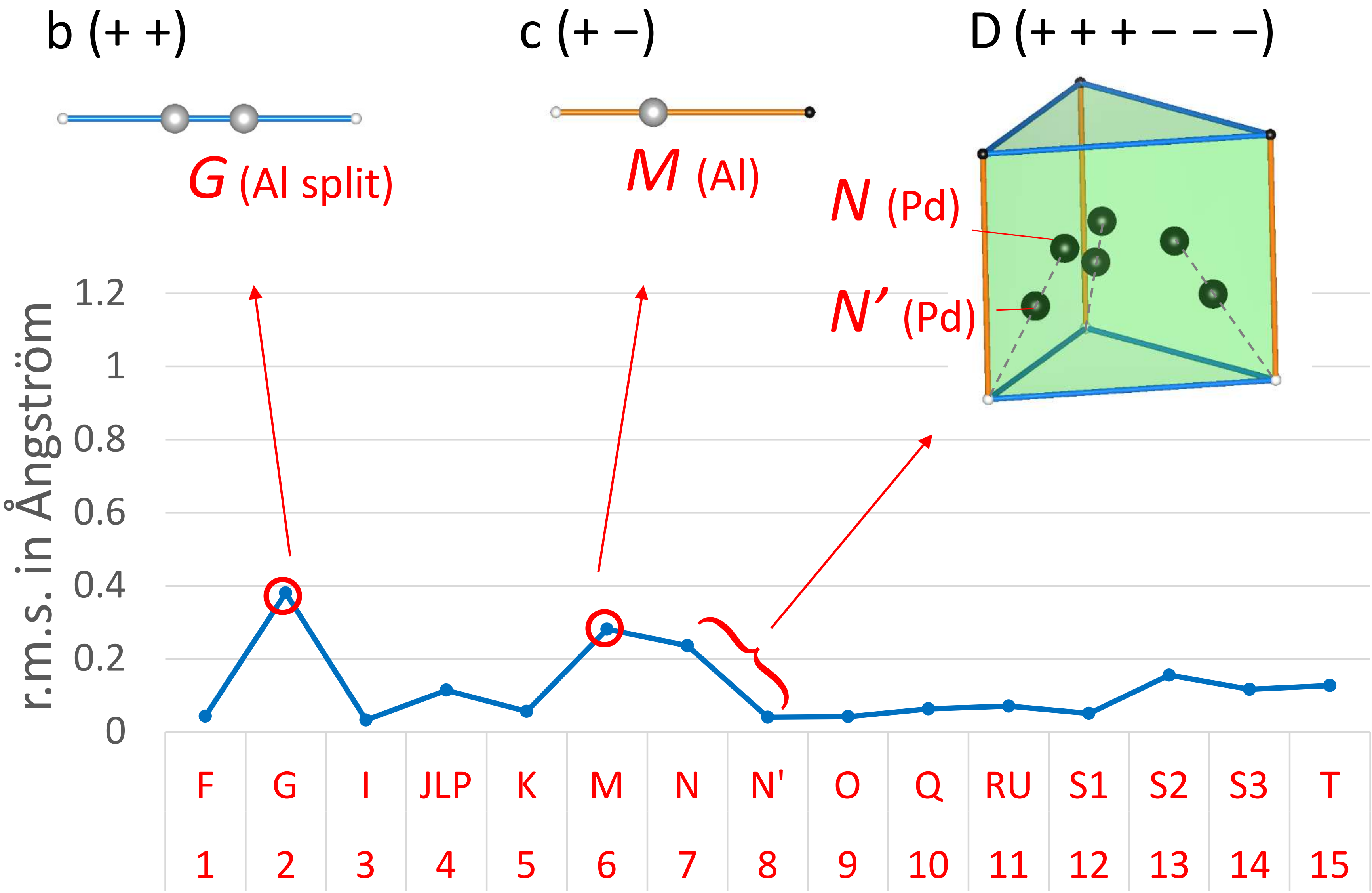


Distance r.m.s. to ideal position

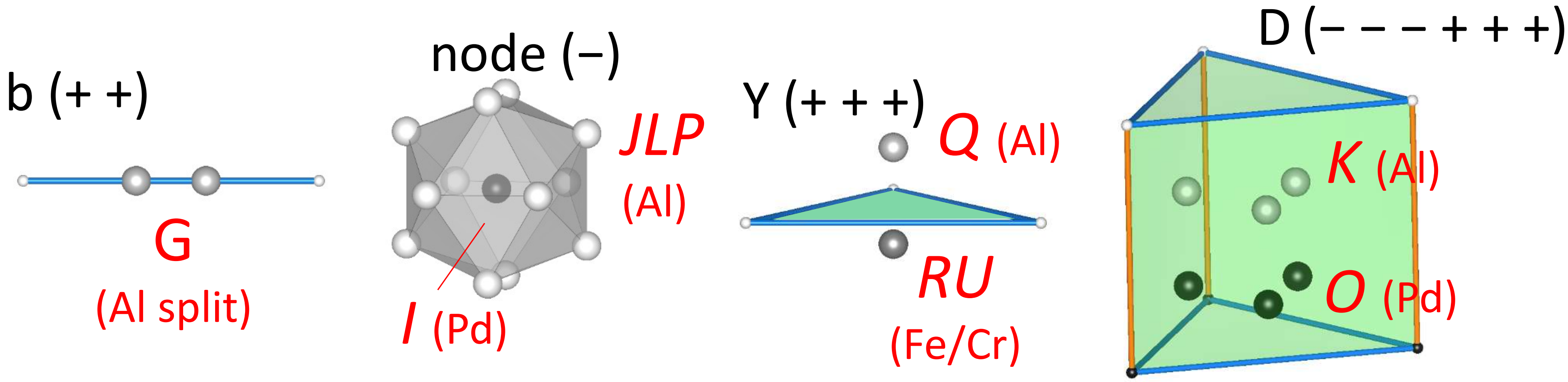


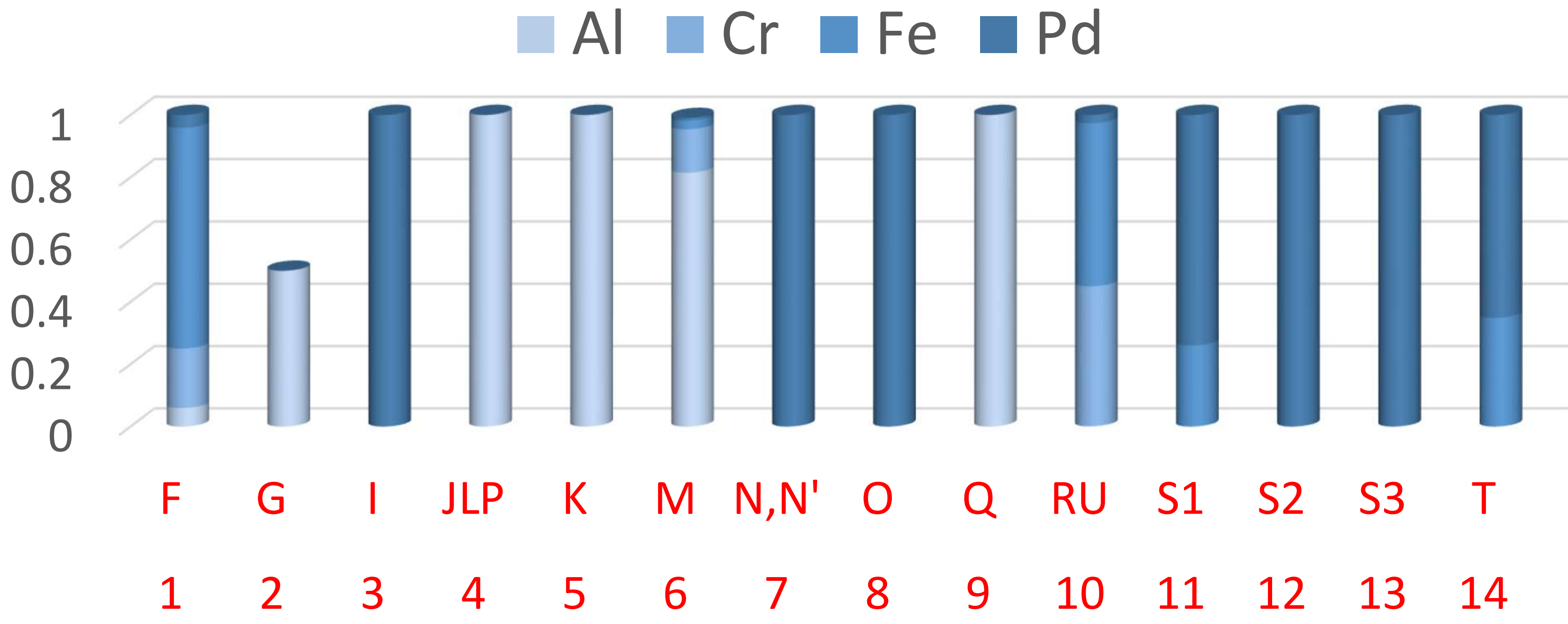


Distance r.m.s. to ideal position



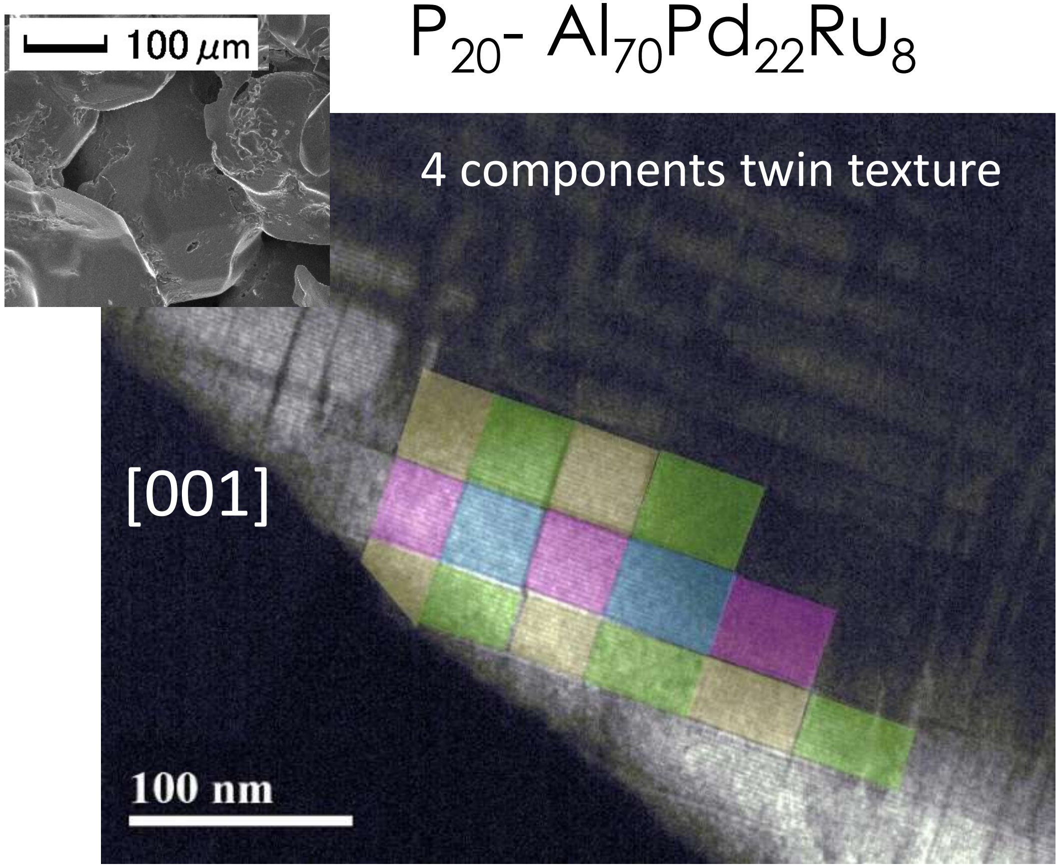
On-site chemistry



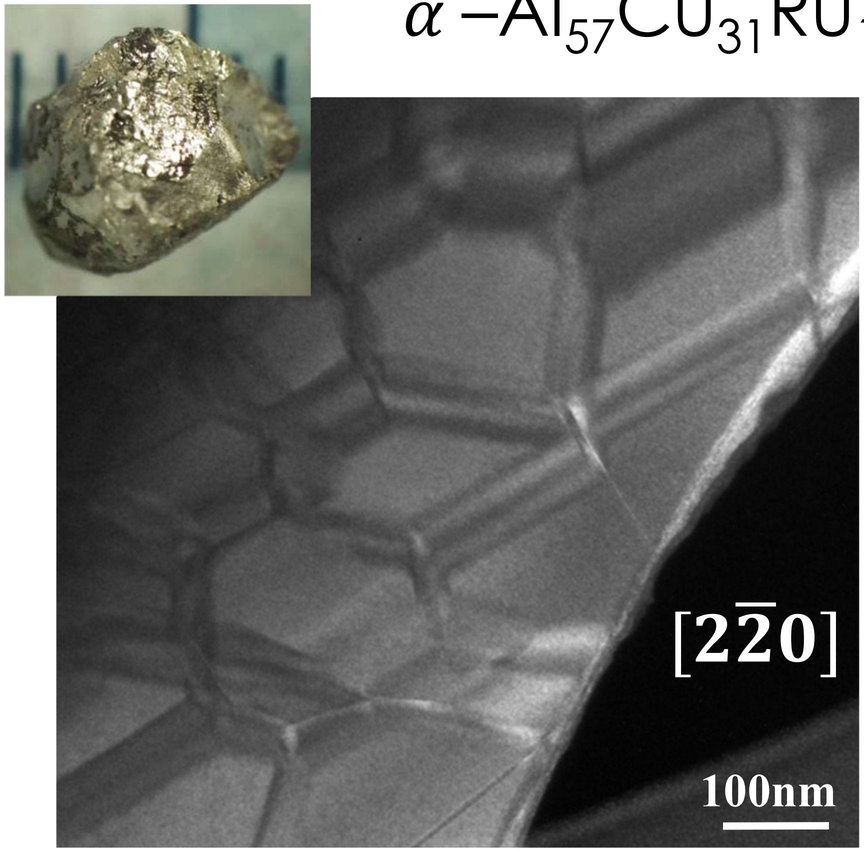


§ Microscopic twinning

P_{20}- $Al_{70}Pd_{22}Ru_8$



α –$Al_{57}Cu_{31}Ru_{12}$

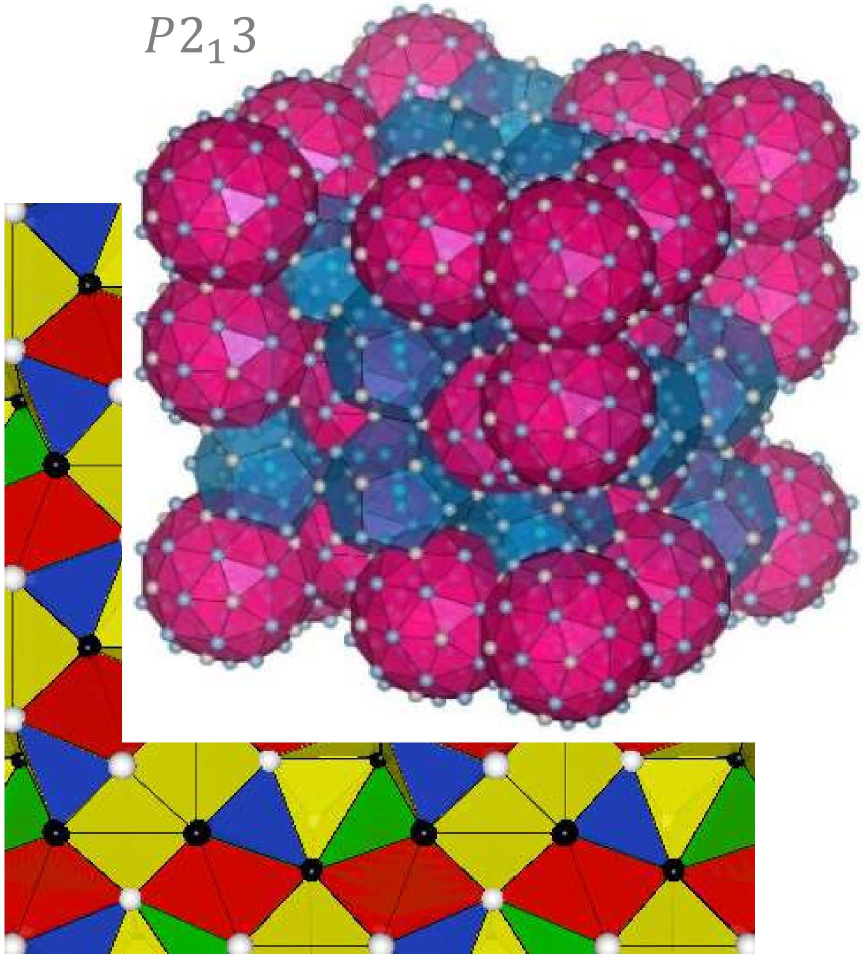


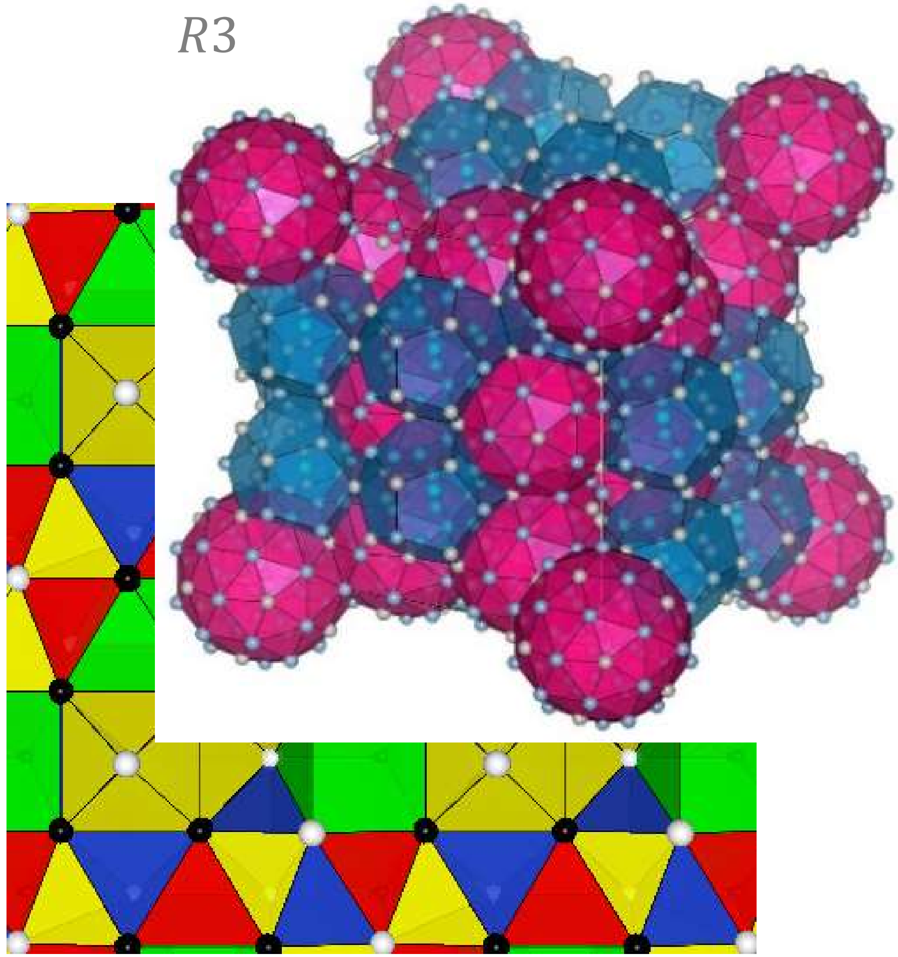
Space group $Pm\bar{3}$
$a \cong 20.3$Å
(3/2 cubic?)

TEM observations – dark field imaging
(Dr. K. Nishimoto)

Space group $Pm\bar{3}$
$a \cong 12.4$Å
(2/1 cubic?)

CCTs for modeling P_{20} phase



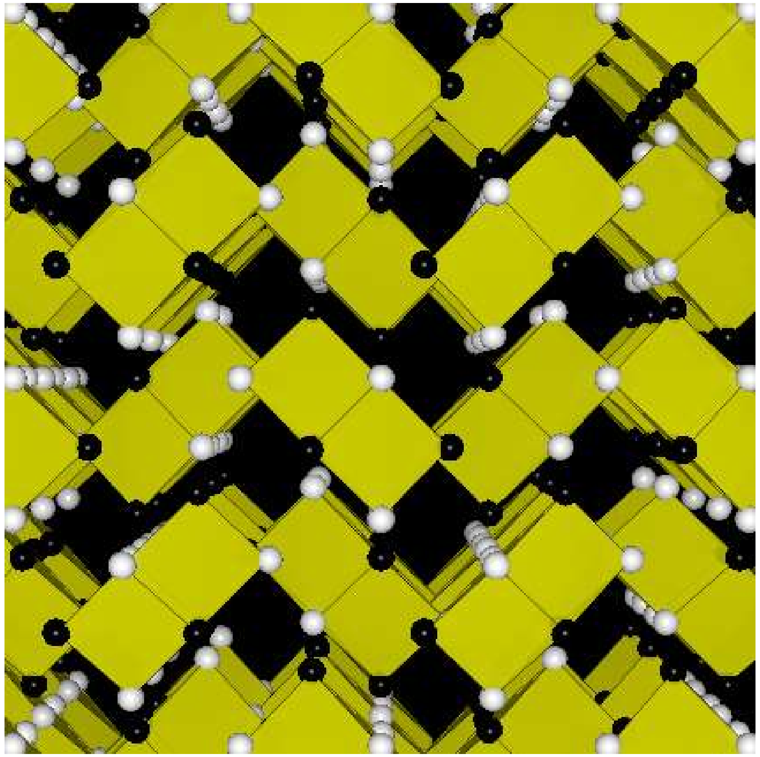


3/2 cubic ($P2_13$)

$(3/2)^3$ rhombohedral ($R3$)

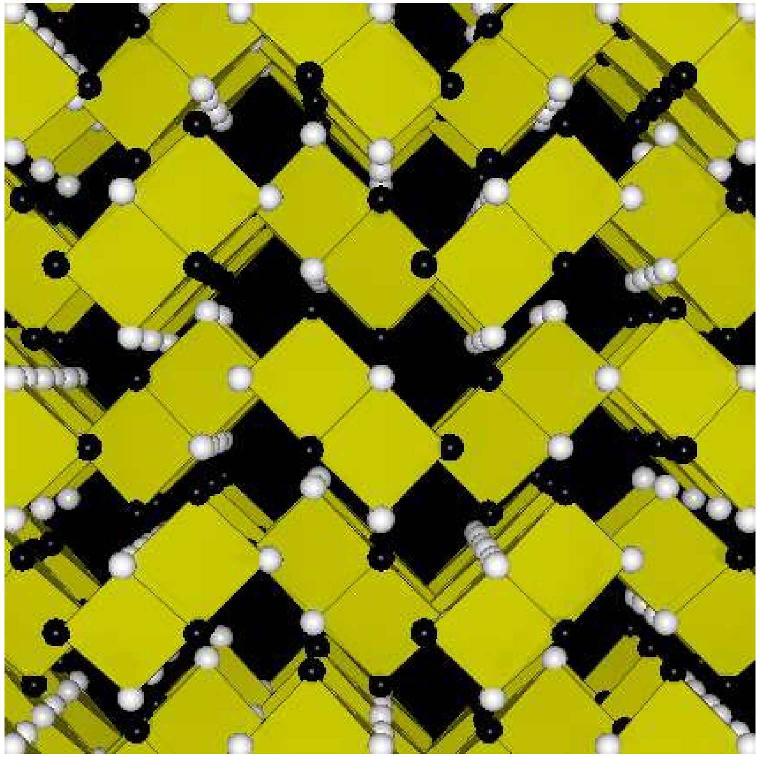
Flip of A_6-unit in 3/2 cubic struc.

A_6 units on F.C.C. lattice



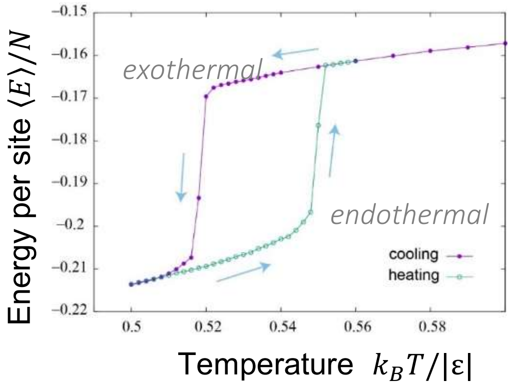
3/2 cubic ($P2_13$)

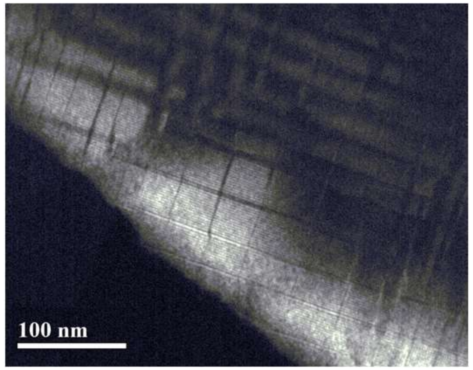
→ *Flip one out of four A_6 units*

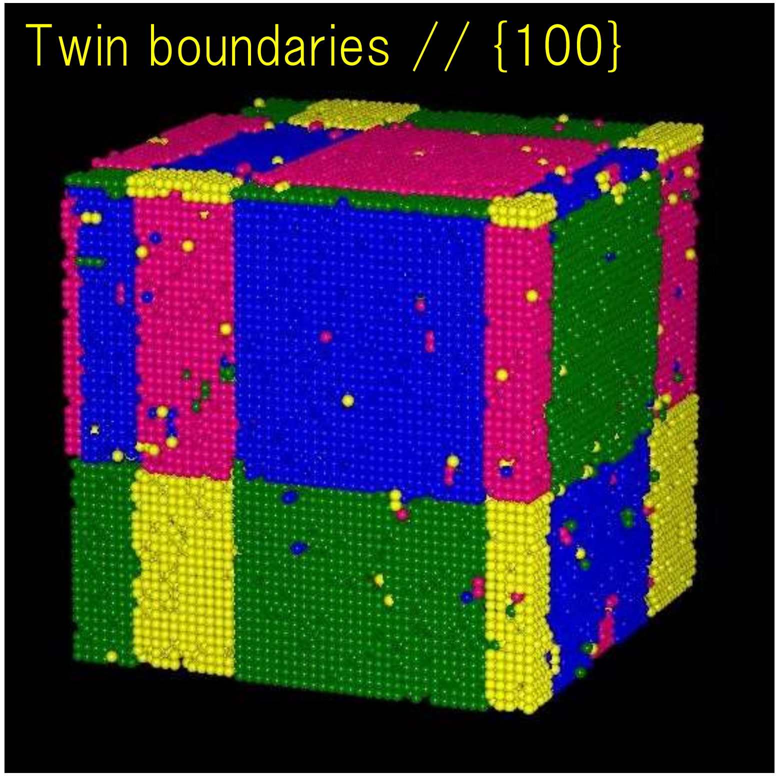


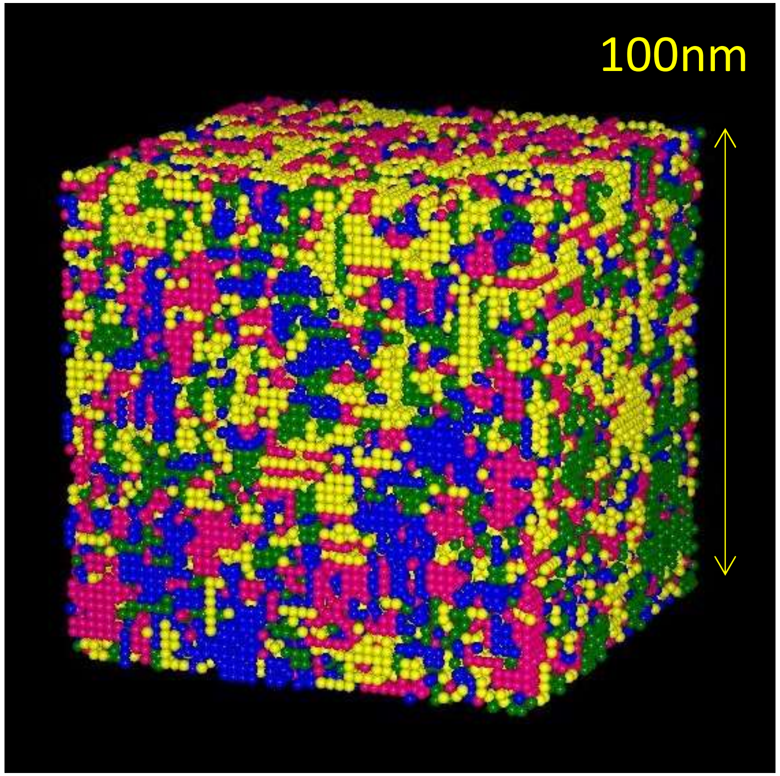
$(3/2)^3$ rhombohedral ($R3$)

Monte-Carlo simulation









$k_B T$ = 0.52
(50,000mcs)
Ordered

$k_B T$ = 0.53
Disordered (up to 500,000 m.c.s.)

Conclusions

Future prospects

Proof of the twinning transition

Structure of twin boundary

Formation and stabilization

New structures, new compounds

etc.

Acknowledgments

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