

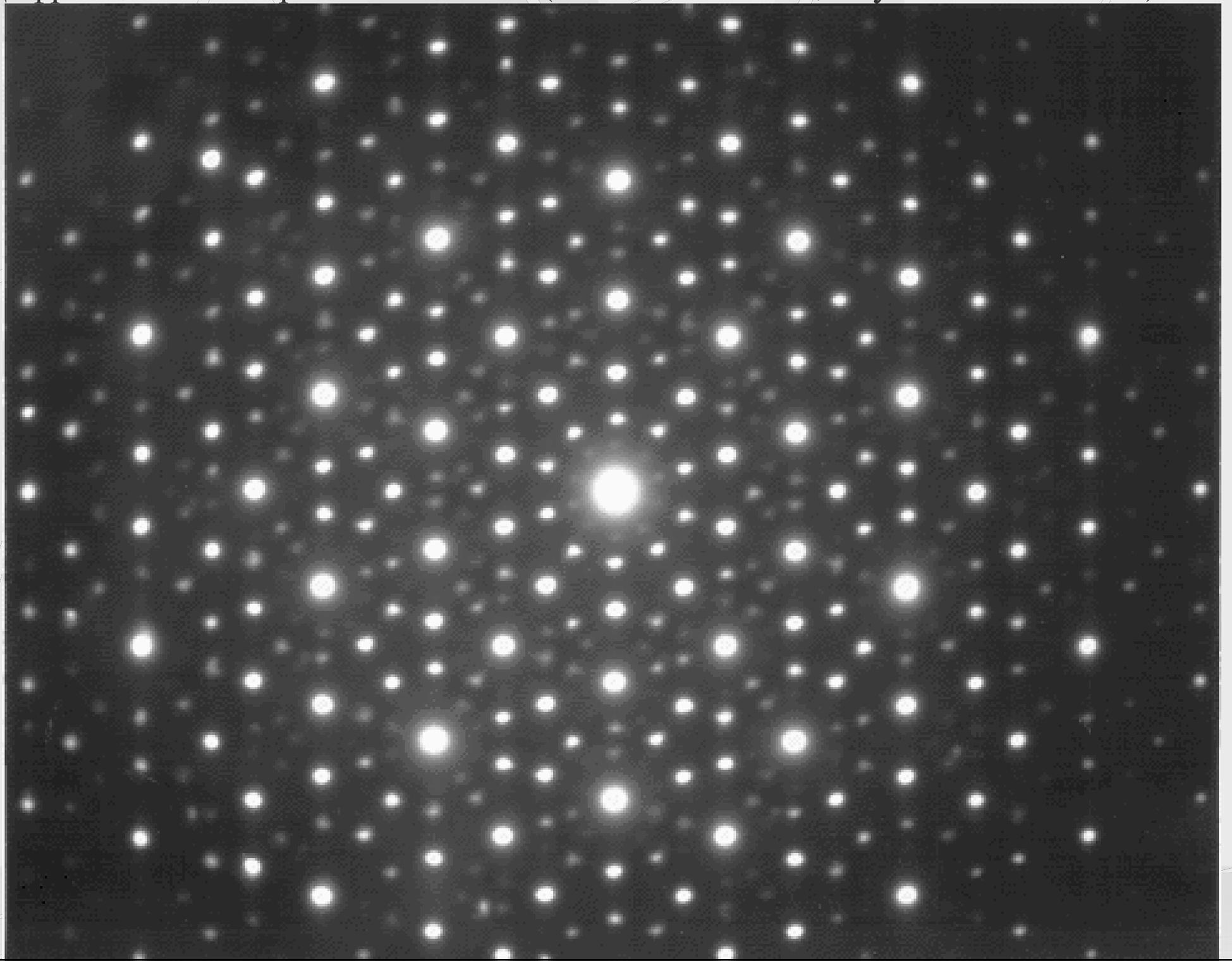
Квазикристаллы и их аппроксиманты

В.Е. Дмитриенко, В.А. Чижиков

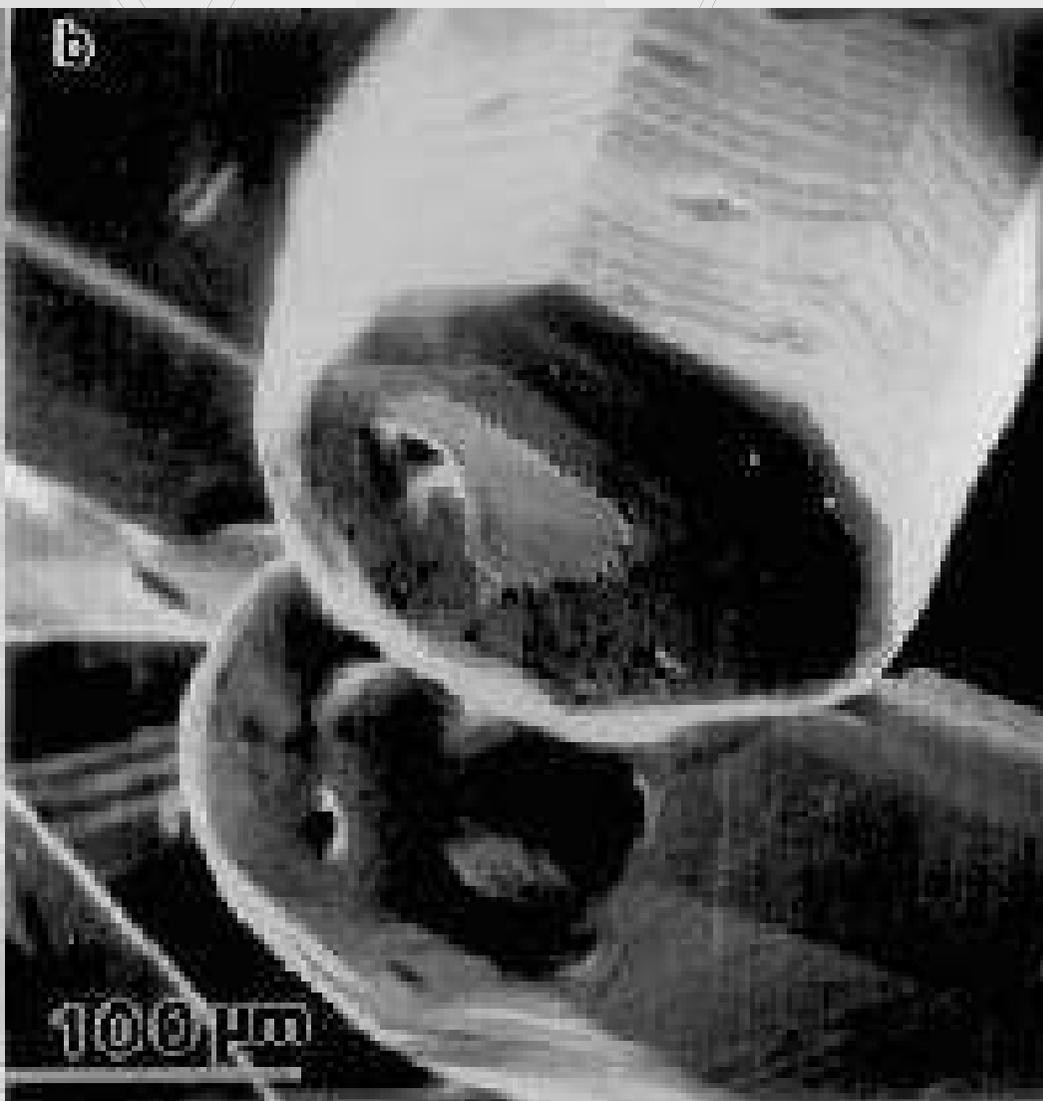
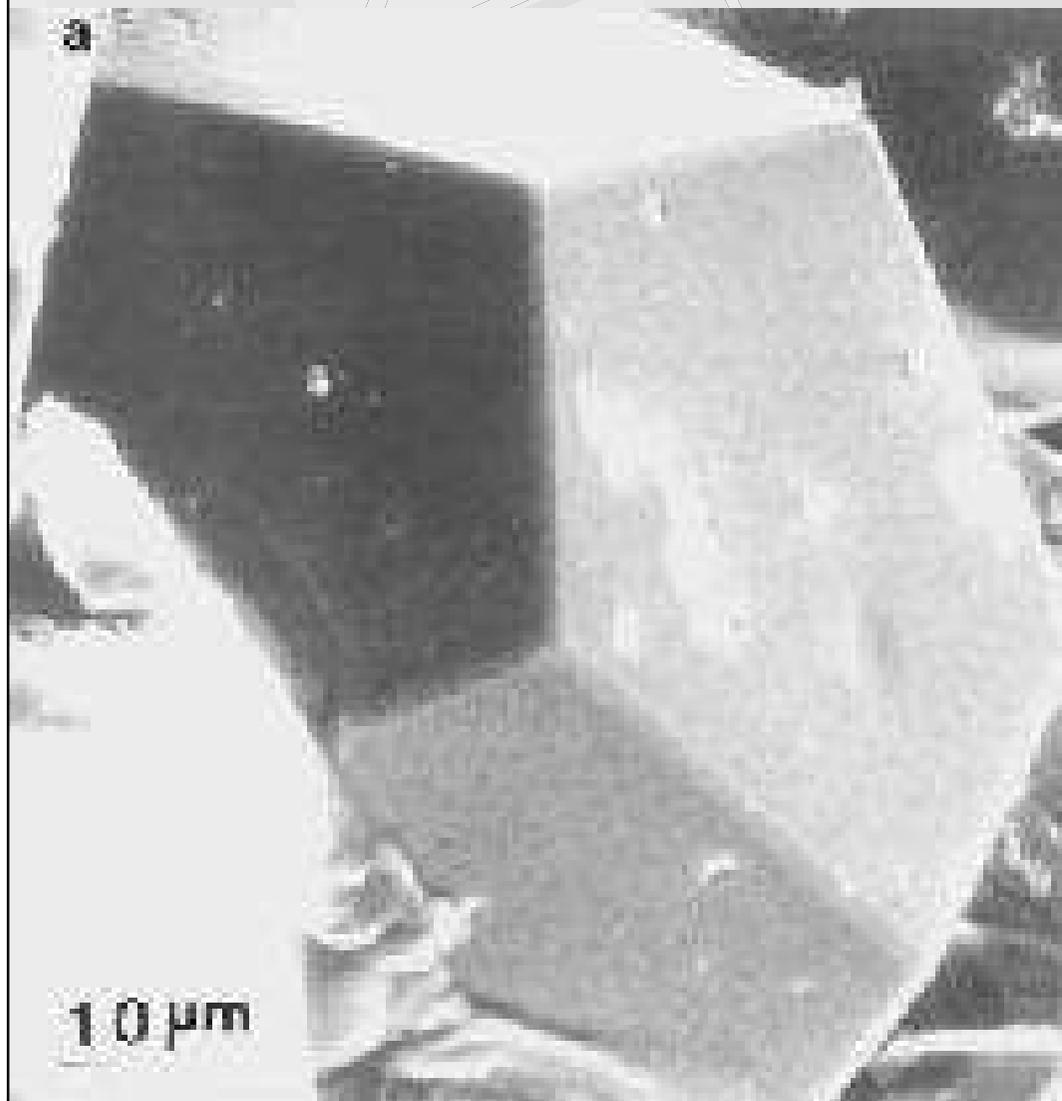
Институт кристаллографии им. А.В.Шубникова

1. Введение
2. Аперриодичность и некристаллографическая симметрия
3. Структурные особенности (самоподобие, кластеры, ...)
4. Аппроксиманты ($MnSi$ со структурой $B20$, $BC8$ фаза кремния)
5. Рост квазикристаллов

Дифракционная картина с осью 10 (Schechtman et al., Phys.Rev.Lett. 1984)

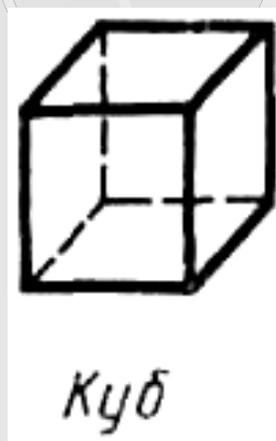
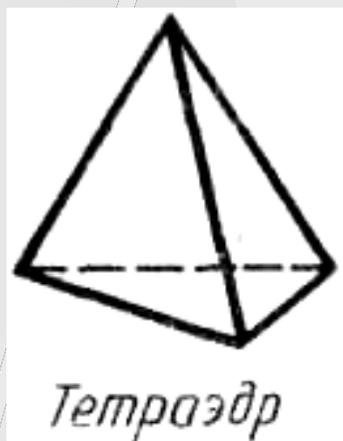


Моноквазикристаллы: икосаэдрический и декагональный

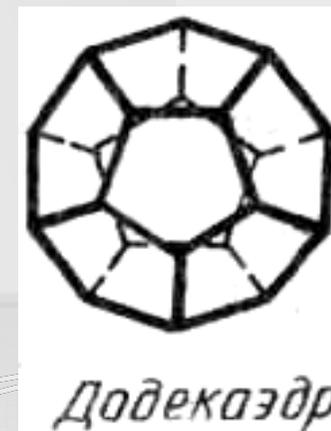


Кристаллографические и некристаллографические точечные симметрии

● Кристаллографические



● Некристаллографические



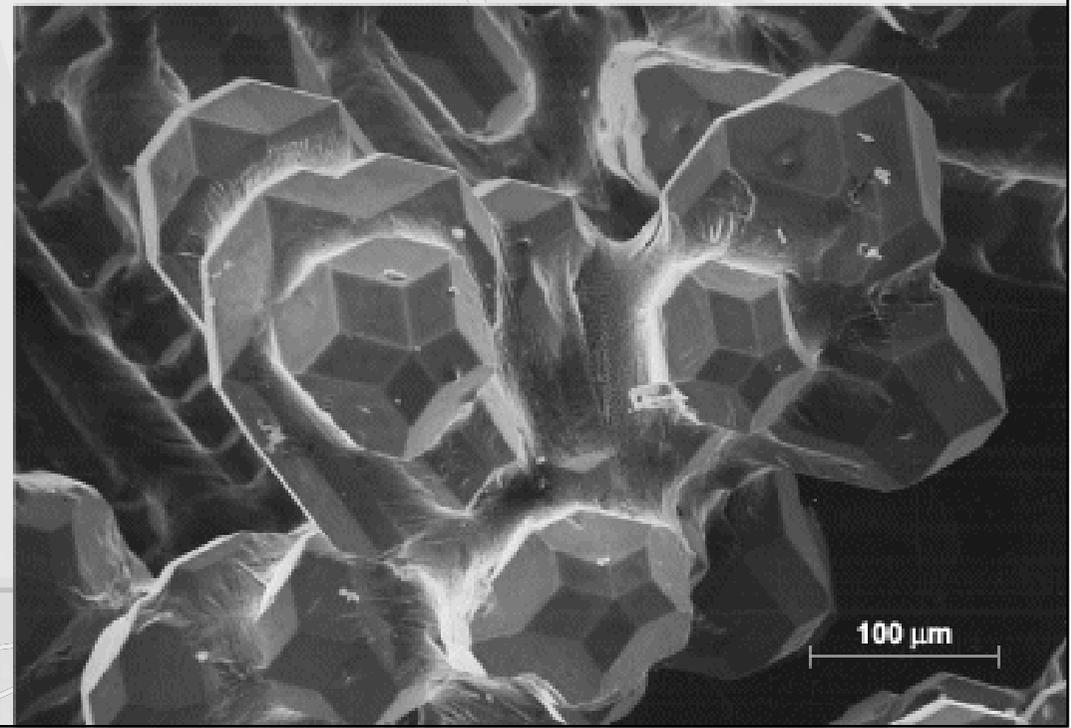
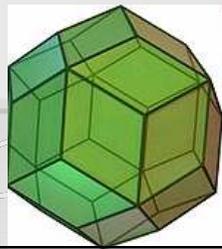
Немного истории...

- Правильные многогранники были известны еще в Древней Греции.
- Придумать правильные многогранники, по-видимому, было нетрудно: часть из них — это формы природных кристаллов. Например, монокристалл поваренной соли (NaCl) — это куб.
- Существует предположение, что додекаэдр древние греки увидели, рассматривая кристаллы пирита (FeS_2), **аппроксимант!** Имея додекаэдр, несложно получить икосаэдр: его вершинами являются центры граней додекаэдра.
- У древнегреческого мыслителя Платона четыре многогранника олицетворяли четыре стихии:
 - ◆ **тетраэдр — огонь,**
 - ◆ **куб — землю,**
 - ◆ **октаэдр — воздух,**
 - ◆ **икосаэдр — воду,**
- ◆ А **додекаэдр** олицетворял **ВСЁ МИРОЗДАНИЕ.**

Экспериментально наблюдались:

- икосаэдрические: оси 5,3,2, плоскости m
- пентагональные: ось 5
- октагональные: ось 8
- декагональные: ось 10
- додекагональные: ось 12

триаконтаэдр



периодическая, ..., аperiodическая

- периодическая: $f(x) = \sum f_n \exp(inx)$

- квазипериодическая:

$f(x) = \sum_{n_1, \dots, n_m} f_{n_1, \dots, n_m} \exp[ix(n_1 k_1 + \dots + n_m k_m)]$, т.е. несколько взаимно несоизмеримых периодов

Такую функцию можно представить как сечение **многомерной периодической функции**

$f(x_1, \dots, x_m) = \sum_{n_1, \dots, n_m} f_{n_1, \dots, n_m} \exp[i(n_1 x_1 + \dots + n_m x_m)]$

линией, заданной уравнениями $x_1 = k_1 x, \dots, x_m = k_m x$

- почти периодическая: $\mathcal{M} = \infty$

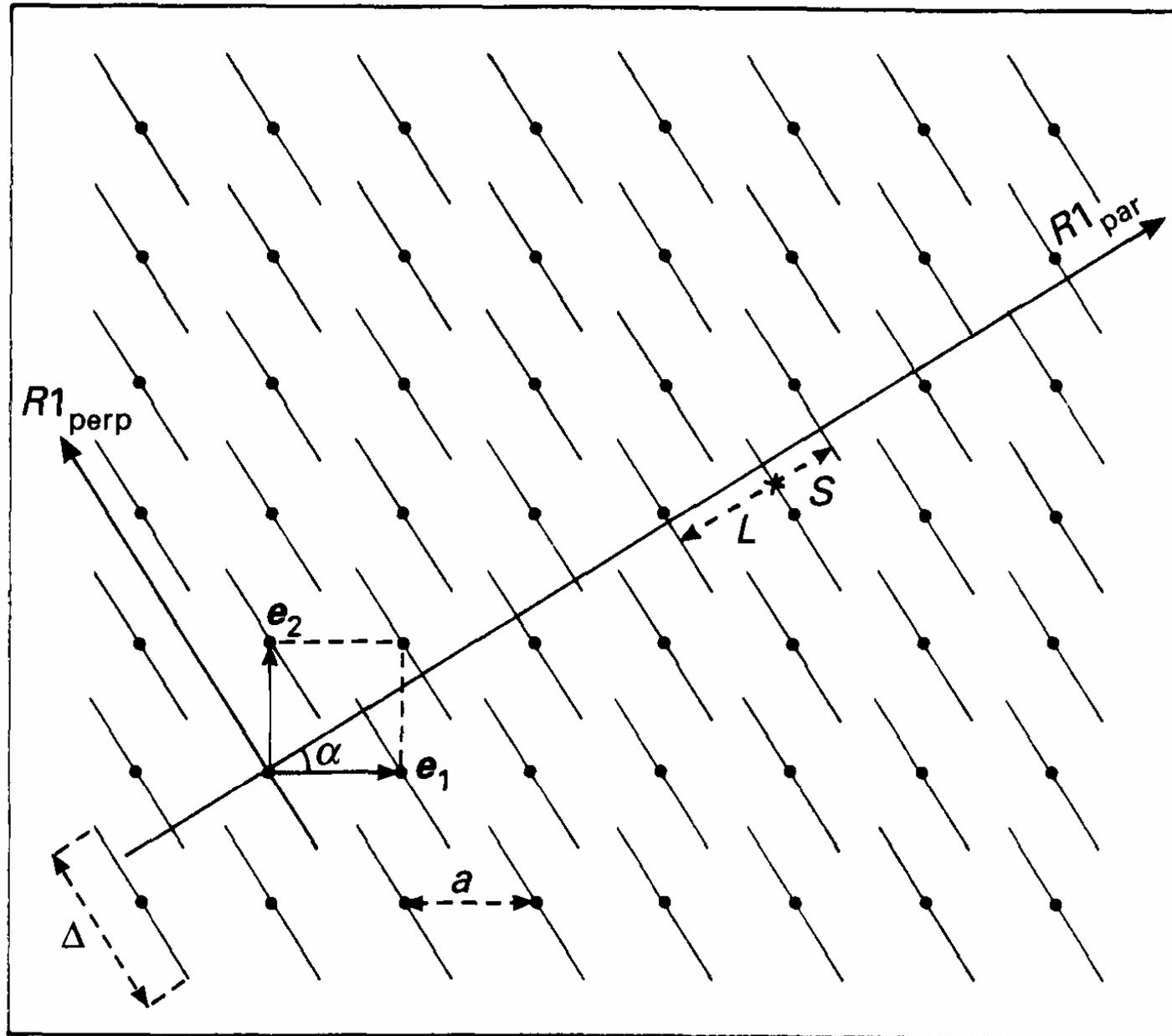


FIG. 1.30 Illustration of the cut-projection method. The basis associated with the 2-dim square lattice is a single line segment perpendicular to the physical 1-dim space. The cut of this 2-dim structure by R_{par} is a Fibonacci chain.

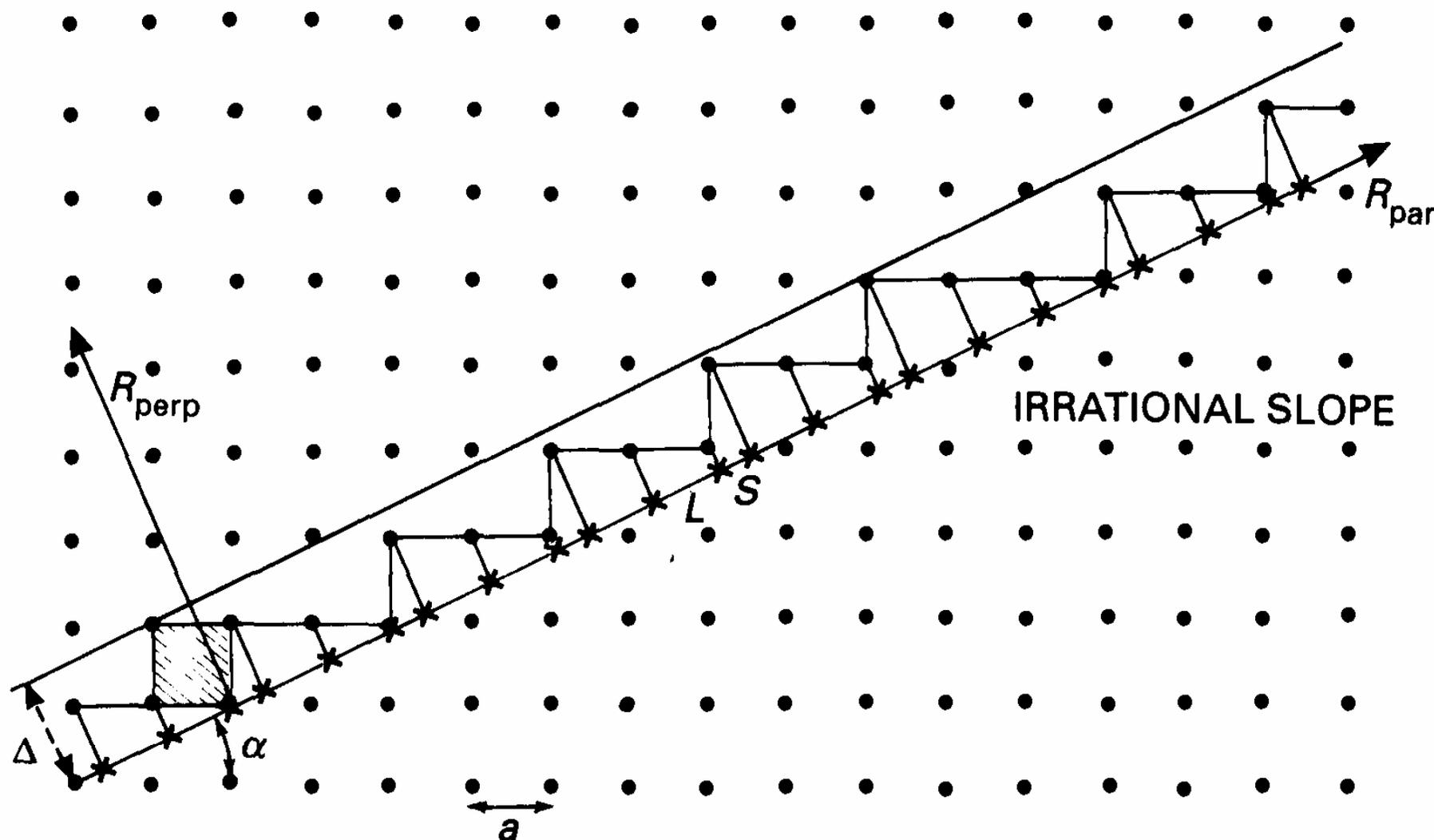


FIG. 1.28 A 1-dim illustration of the strip/projection method. The slope of R_{par} is irrational. Sites of the portion of the square lattice inside the strip project on R_{par} in a perfectly ordered non-periodic structure made of two tiles of incommensurate sizes. With a slope of R_{par} equal to τ , the Fibonacci chain is obtained.

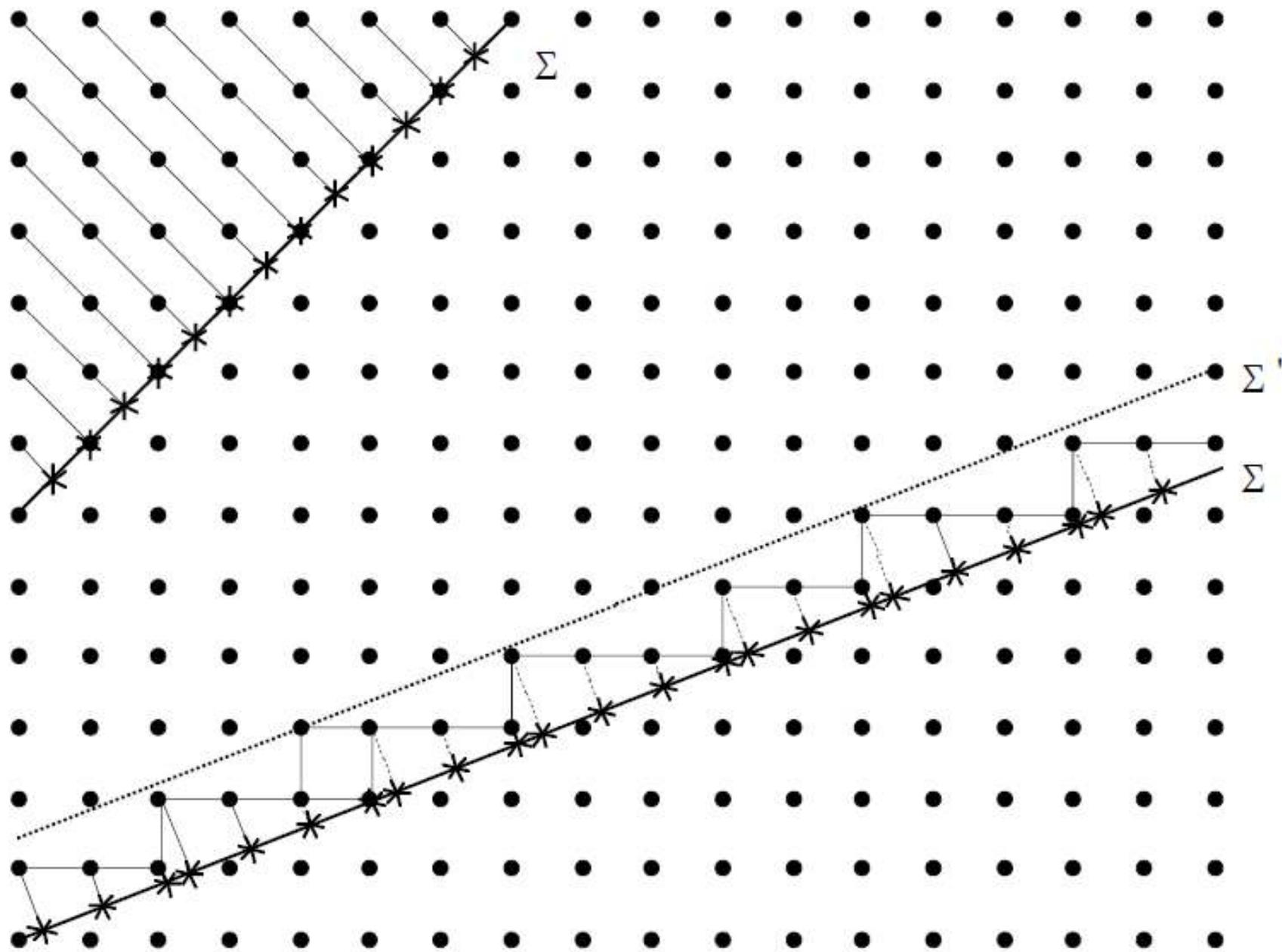


Figure 2.9. Illustration in $d + n = 2$ dimensions of the crystallography of periodically modulated and quasicrystalline materials. A 2D square lattice projects onto a line Σ either as a 1D periodic structure when the slope of Σ is rational (upper left corner) or as an incommensurate aperiodic structure when the slope is irrational (central part).

Аппроксиманты Фибоначчи

1/0: A.A.A.A.A.A.A.A подстановка: $A \rightarrow AB, B \rightarrow A$

1/1: AB.AB.AB.AB.AB.AB.AB.AB.AB

2/1: ABA.ABA.ABA.ABA.ABA.ABA.ABA

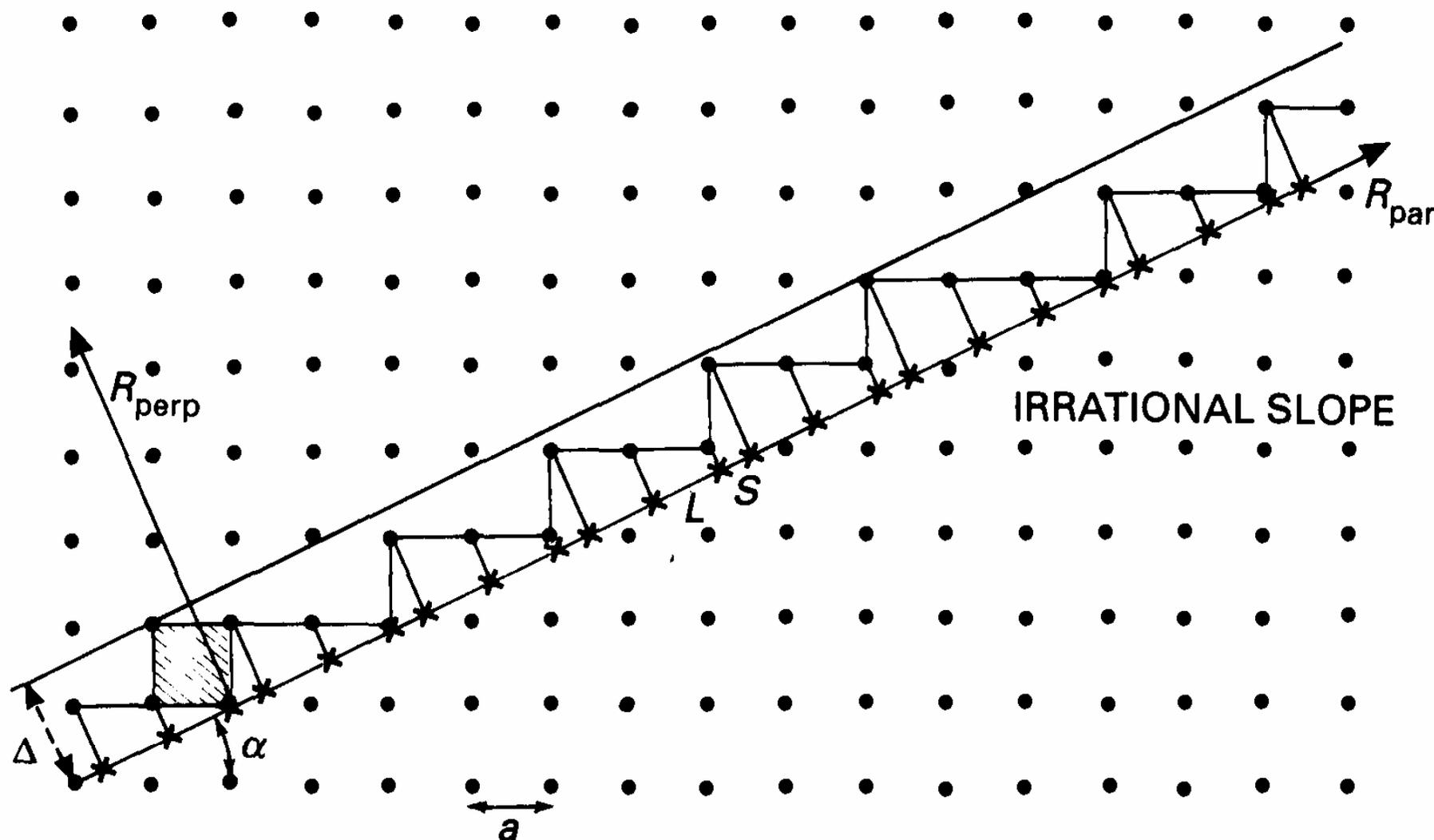
3/2: ABAAB.ABAAB.ABAAB.ABAAB

5/3: ABAABABA.ABAABABA.ABAABABA

τ : ABAABABAABABAABABAABABAABABAAB

Числа Фибоначчи: $F_{n+2} = F_{n+1} + F_n, F_0 = 0, F_1 = 1;$

0,1,2,3,5,8,13,21,34,55,89,... $\tau = (1 + 5^{1/2})/2 = 1.618034$



$$R_{\text{par}} = m + \tau n, \quad R_{\text{perp}} = \tau m - n;$$

FIG. 1.28 A 1-dim illustration of the strip/projection method. The slope of R_{par} is irrational. Sites of the portion of the square lattice inside the strip project on R_{par} in a perfectly ordered non-periodic structure made of two tiles of incommensurate sizes.

With a slope of R_{par} equal to τ , the Fibonacci chain is obtained.

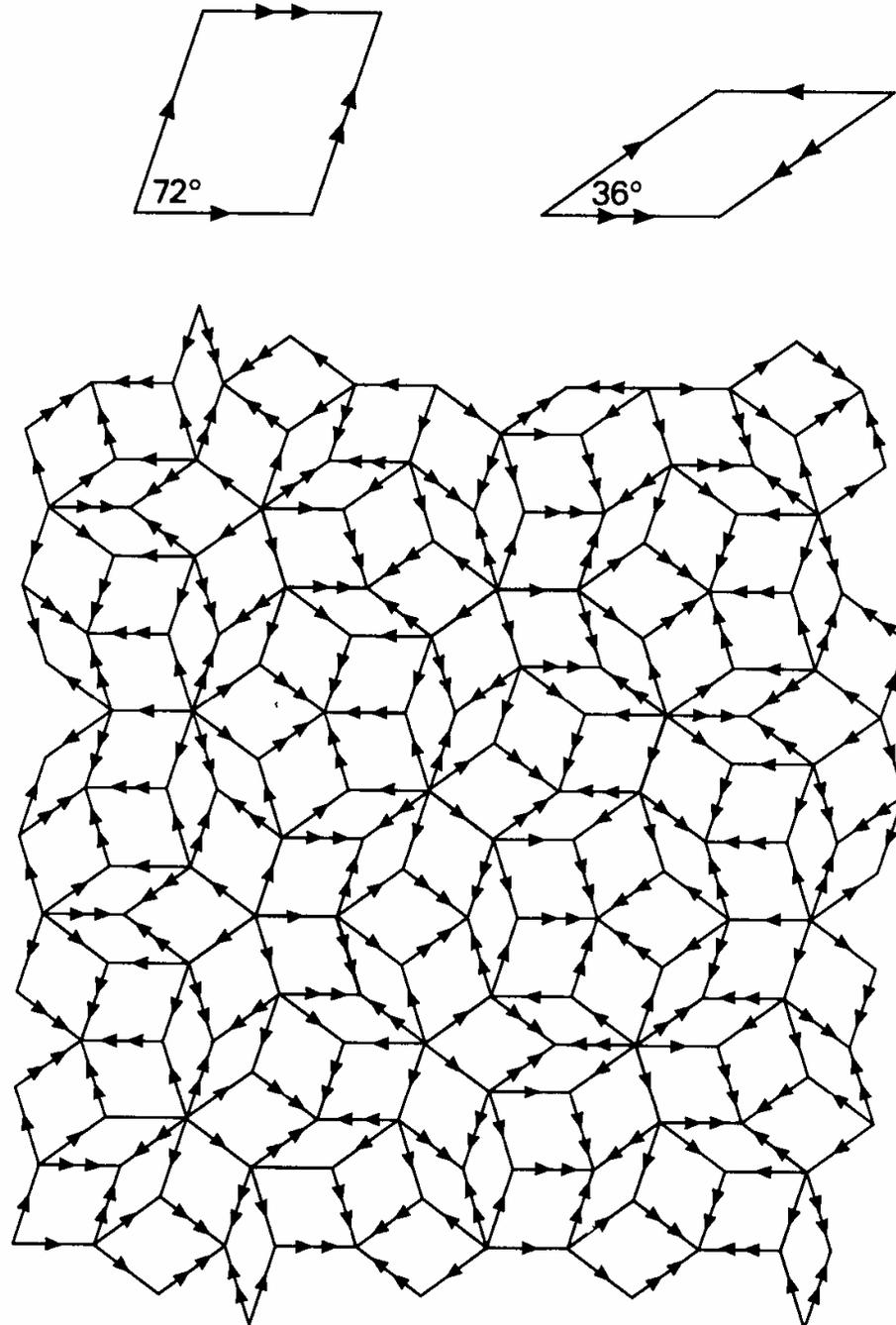


FIG. 1.21 Two-dimensional Penrose tiling with two lozenges as unit cells and edge matching rules (see text).

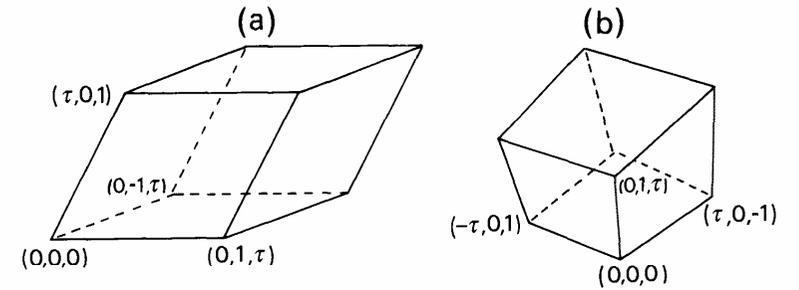


FIG. 1.23 Schematic of (a) prolate and (b) oblate rhombohedra that can be used for 3-dim Penrose tiling. Vertex coordinates are given in a frame of three orthogonal 2-fold axes of a regular icosahedron.

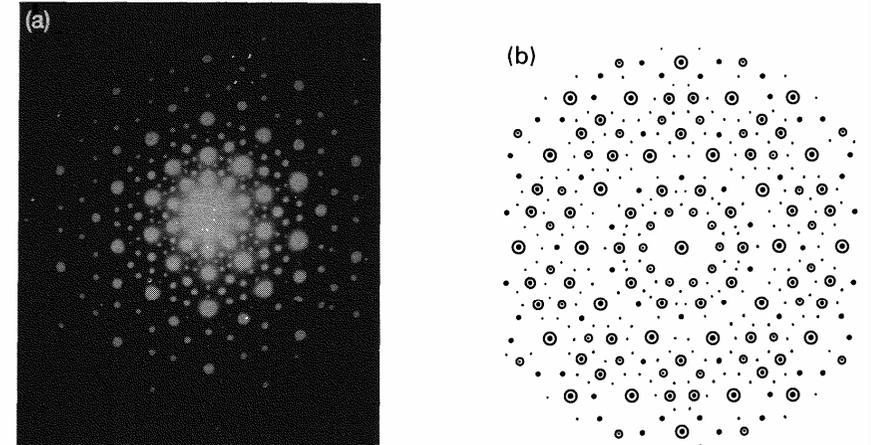


FIG. 1.24 Electron diffraction pattern of an AlMn quasicrystal (5-fold zone axis) (a) compared with the computed Fourier pattern of a 3-dim Penrose tiling (b) and as obtained perpendicular to a 5-fold axis.

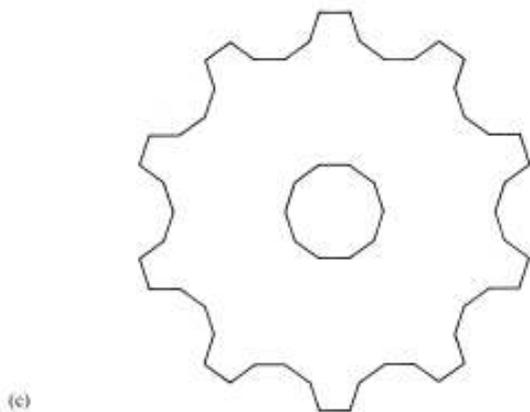
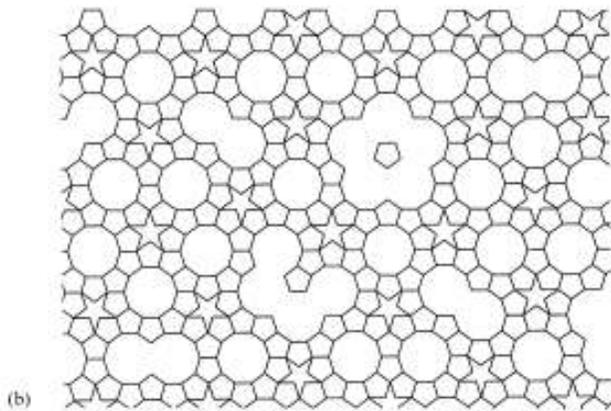
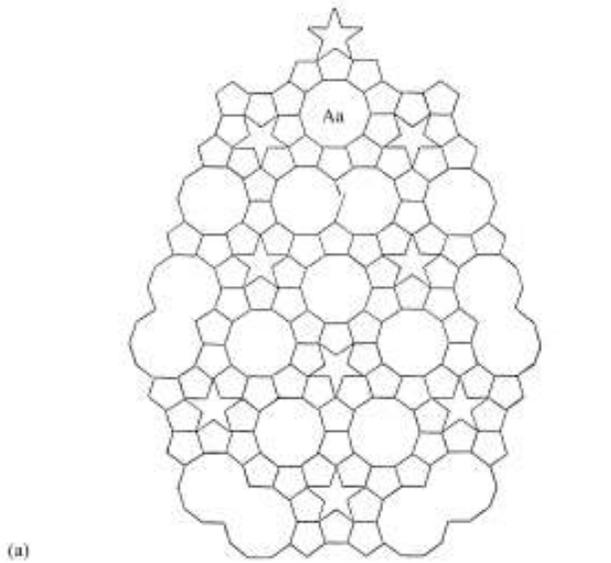


Fig. 2. Kepler's Aa tiling: (a) original patch [2]; (b) computed patch based upon the acceptance domain; (c) acceptance domain.

ab Kepler

Фазонные прыжки атомов

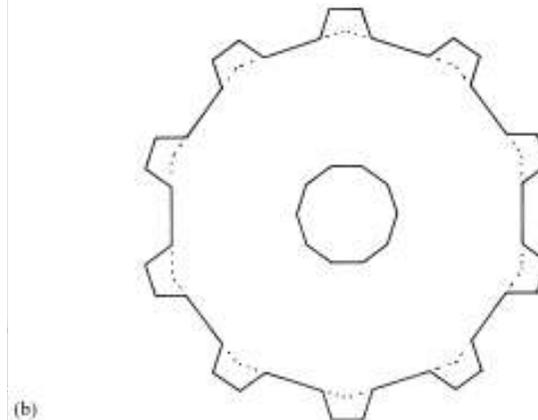
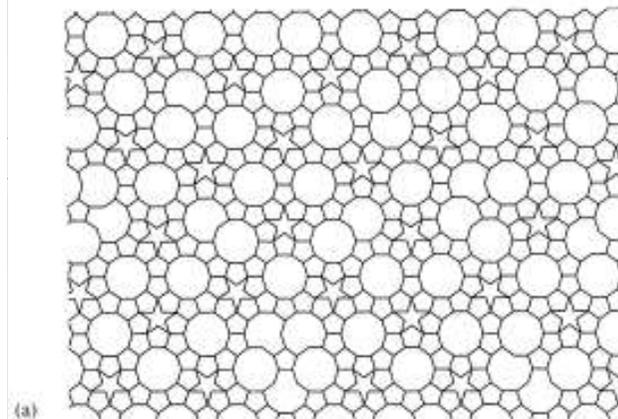


Fig. 3. A modified version of the Aa tiling: (a) tiling; (b) acceptance domain.

Дифракция в квазикристалле

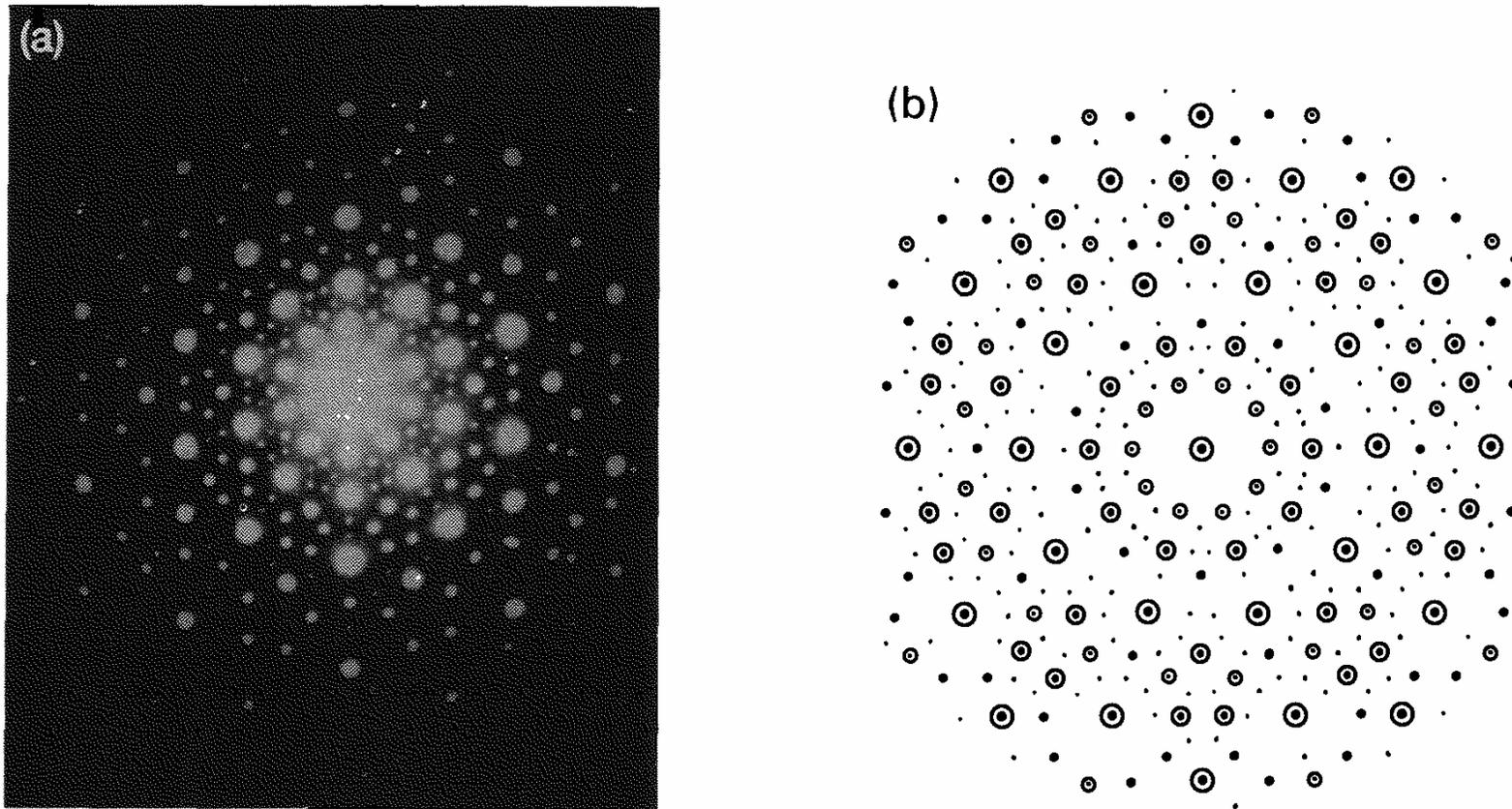


FIG. 1.24 Electron diffraction pattern of an AlMn quasicrystal (5-fold zone axis) (a) compared with the computed Fourier pattern of a 3-dim Penrose tiling (b) and as obtained perpendicular to a 5-fold axis.

$$\mathbf{Q}_{\text{par}} = (m_x + \tau n_x)x + (m_y + \tau n_y)y + (m_z + \tau n_z)z$$

$$\mathbf{Q}_{\text{perp}} = (\tau m_x - n_x)x + (\tau m_y - n_y)y + (\tau m_z - n_z)z$$

Свойства квазипериодических структур

- Каждый «атом» имеет уникальное окружение
- Сколь угодно большие куски повторяются бесконечное число раз
- Понятие симметрии изменяется! Например, при повороте можно совместить сколь угодно большие куски, но не всю структуру.
- Самоподобие (инфляция)
- Фазонная свобода: несчетное множество макроскопически эквивалентных структур
- Дифракционная картина состоит из δ -пикув, но она всюду плотная в обратном пространстве

Где находятся атомы?

Как атомы узнают свои места?

- Аппроксиманты в сплавах с известной кристаллической структурой
- Дифракция нейтронов с изотопным замещением
- Анализ EXAFS (локальное окружение)
- Рентгеноструктурный анализ атомных поверхностей в перпендикулярном пространстве
- Модели роста квазикристаллов

1/1 аппроксимант (Bergman), $a \approx 14 \text{ \AA}$

JEGLIČ *et al.*

PHYSICAL REVIEW B **75**, 014202 (2007)

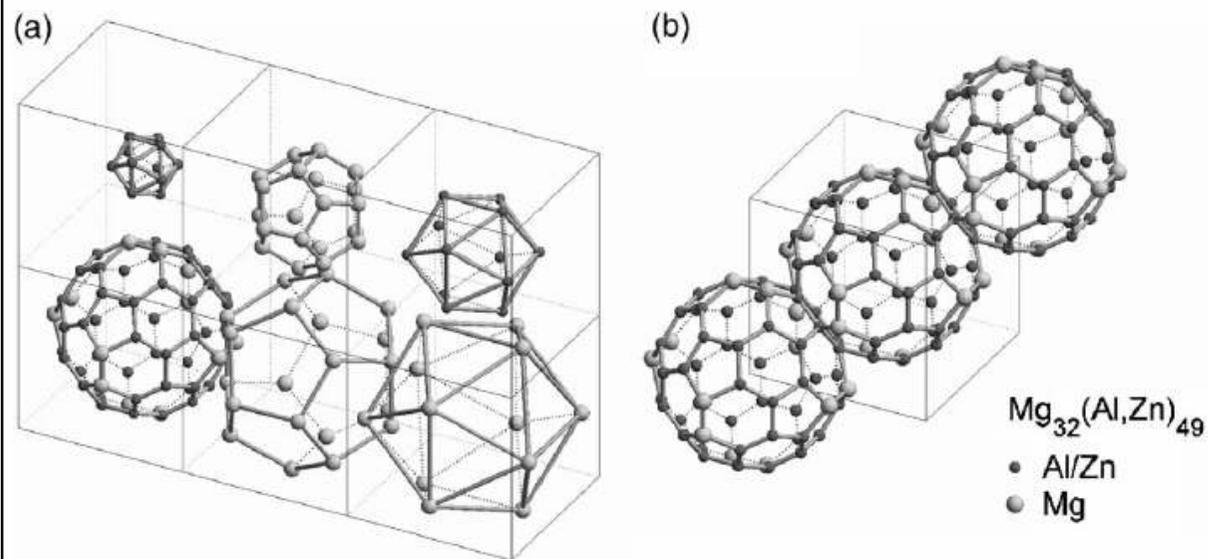


FIG. 7. (a) Six successive shells of the Bergman icosahedral cluster (see text). (b) The structure of the Bergman phase is obtained by a body-centered packing of these clusters by sharing a hexagonal plane of the fourth shell (the soccer ball).

≈ 160 атомов на ОЦК ячейку

1/1 аппроксимант (Маскау), $a \approx 12.5 \text{ \AA}$

SIMONET *et al.*

PHYSICAL REVIEW B 72, 024214 (2005)

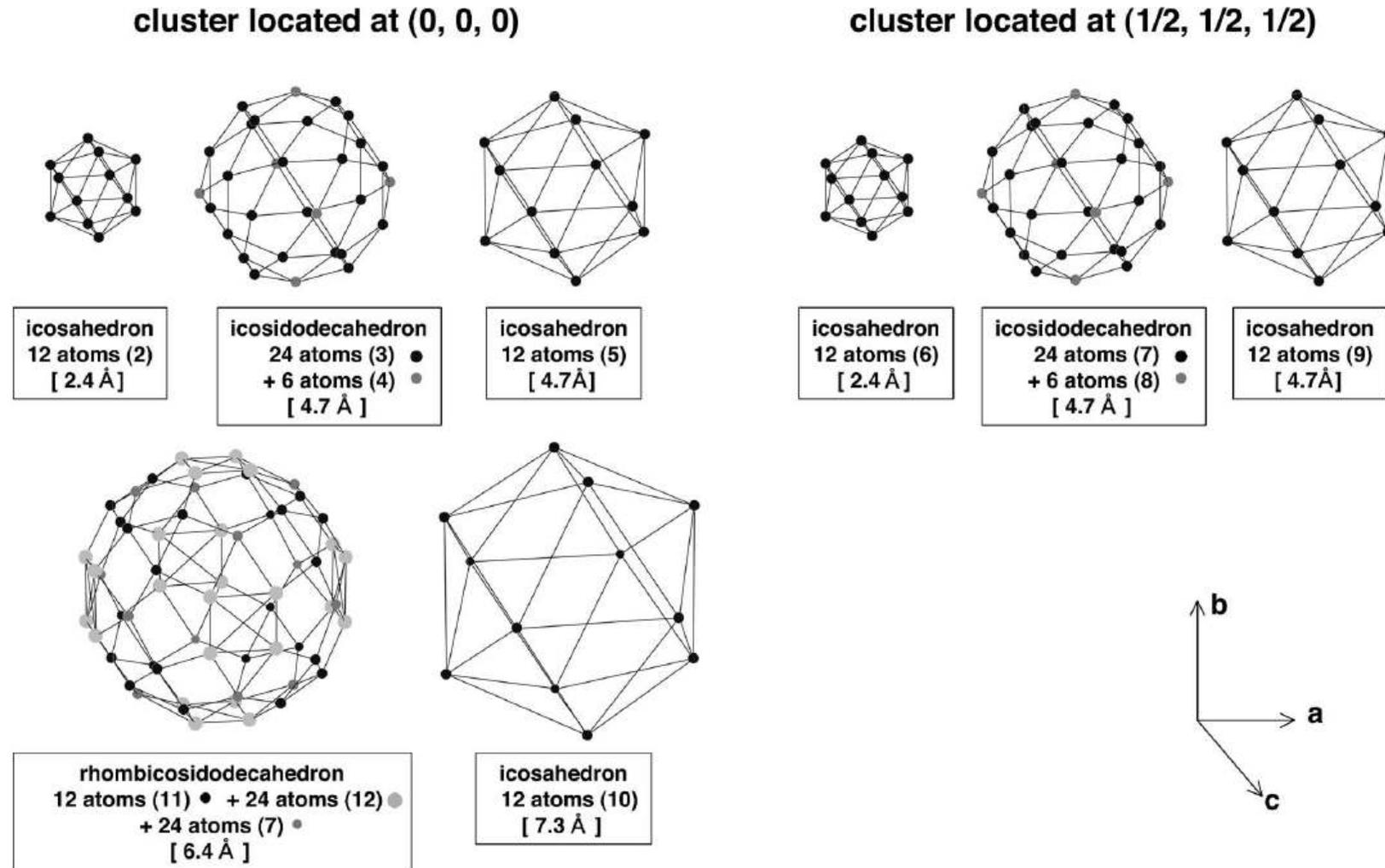
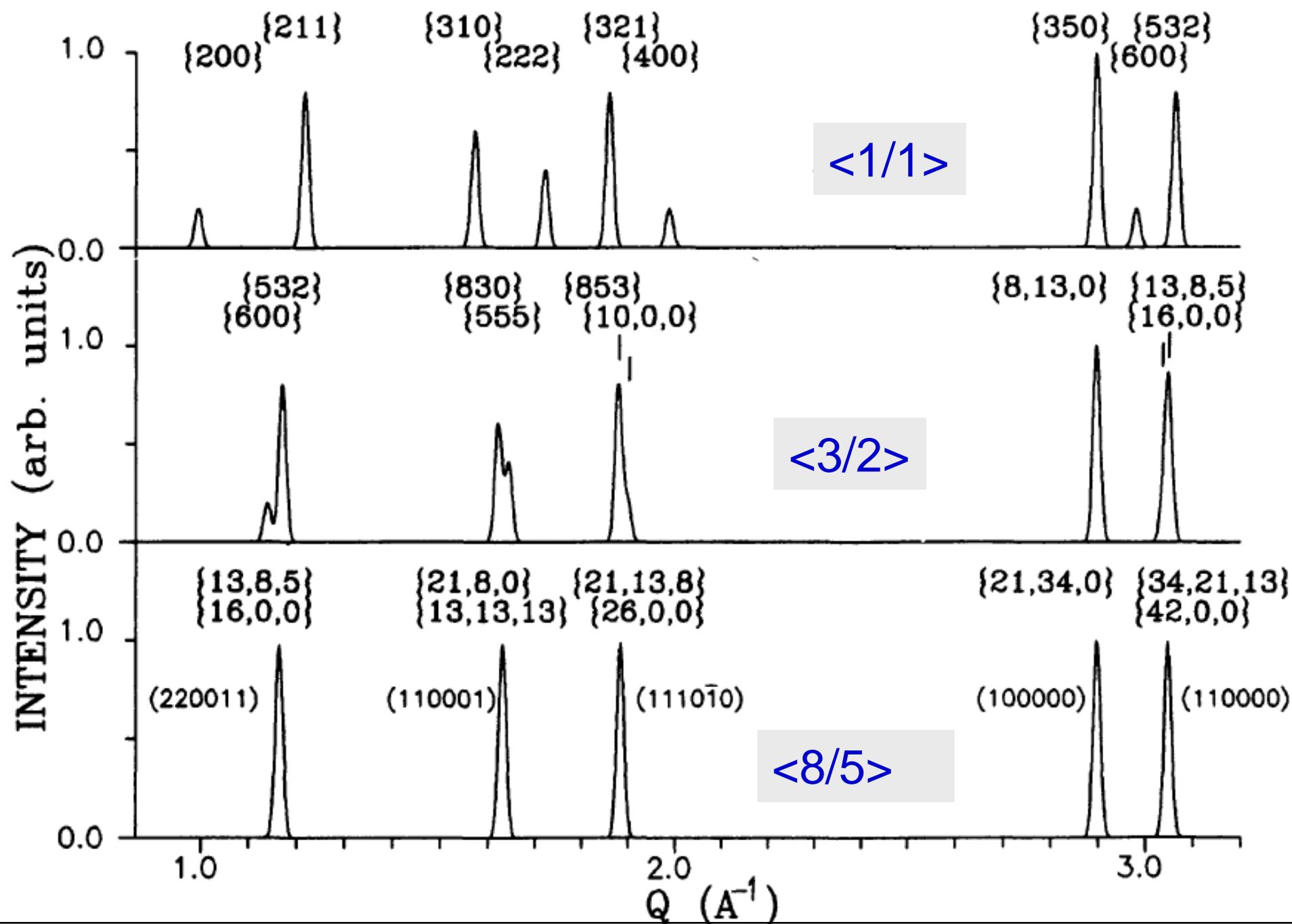


FIG. 2. Atomic structure of the clusters with icosahedral symmetry centered at (0, 0, 0) and (1/2, 1/2, 1/2) in 1/1 approximants in the Al(Si)-Cu-Fe system. For each cluster, the concentric shells with increasing size are shown separately. The crystallographic sites used to build each shell are indicated. Their labels (numbers within parentheses) follow the notations of Tables I and III. The average radius of the shell is indicated. In the α -Al(Si)-Cu-Fe approximant, an additional atom (not represented in the figure) occupies the (0, 0, 0) position and induces an important disorder in the first shell, which loses its icosahedral character. The chemical decoration of these clusters is given in Table I.

Дифракция в кубических аппроксимантах



Электронная дифракция в квазикристалле

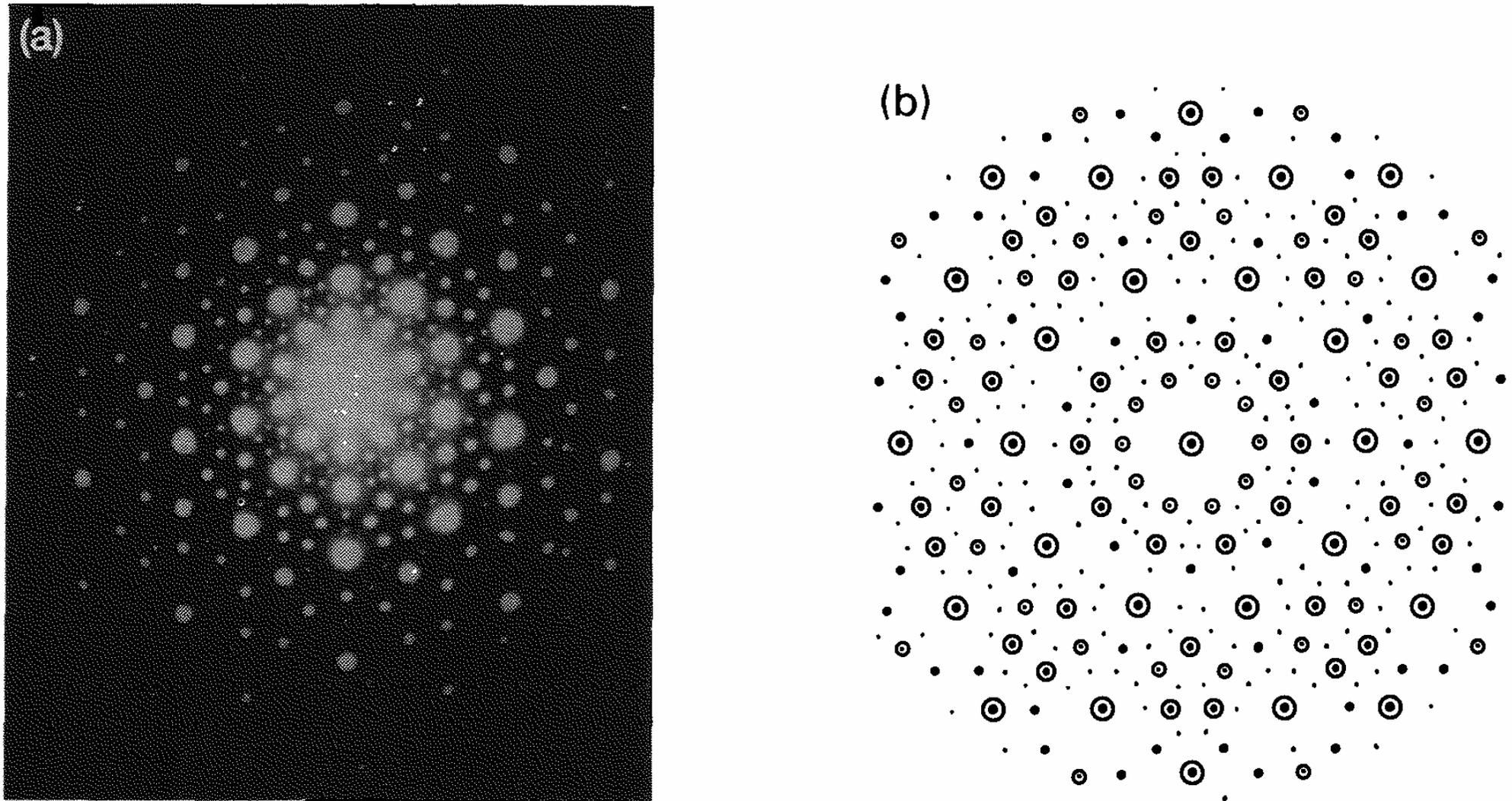


FIG. 1.24 Electron diffraction pattern of an AlMn quasicrystal (5-fold zone axis) (a) compared with the computed Fourier pattern of a 3-dim Penrose tiling (b) and as obtained perpendicular to a 5-fold axis.

Электронная дифракция в кубических аппроксимантах

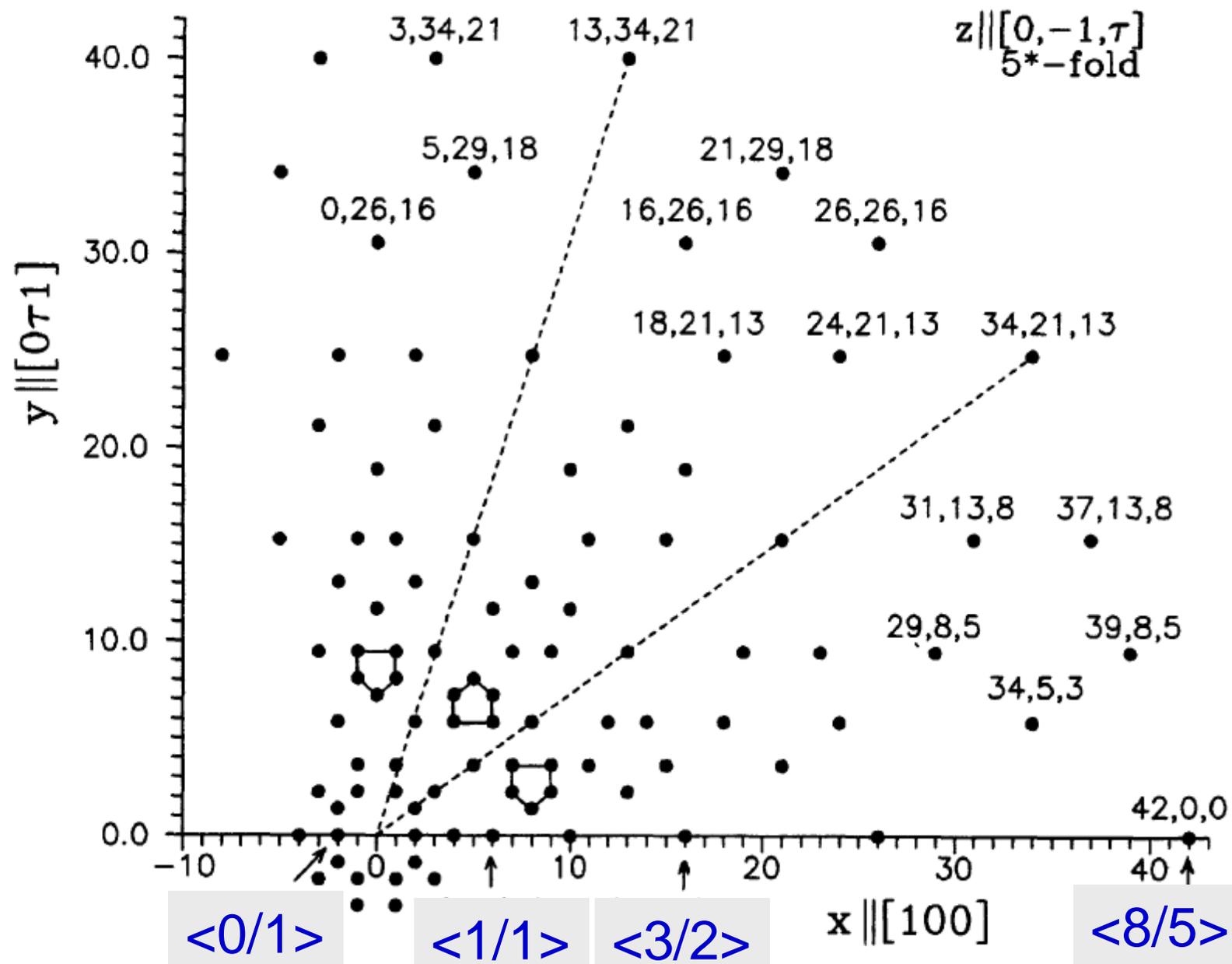


Fig. 3. — Universal pseudo-fivefold electron-diffraction pattern of the Fibonacci crystals

Сравнение с экспериментом AlMnSi

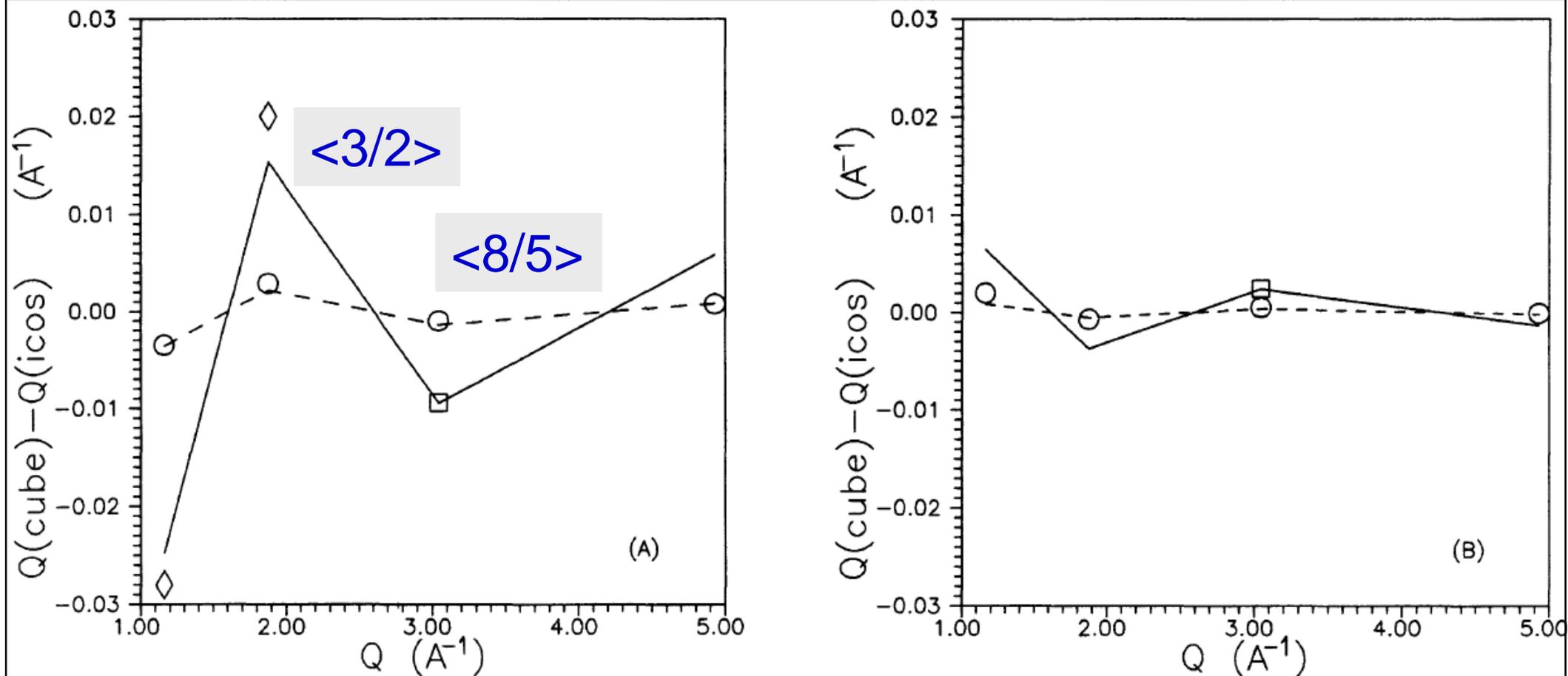


Fig. 7. — The deviations of cubic reflections from their icosahedral positions in different Fibonacci crystals : (A) for the twofold $\{2 F_i, 0, 0\}$ reflections and (B) for the pseudo-twofold $\{F_{i+1}, F_i, F_{i-1}\}$

Определение пространственных групп кубических аппроксимантов и фаз рефлексов из теории Ландау

2. Попытаемся теперь установить, к каким именно кубическим пространственным группам могут принадлежать рассматриваемые структуры. Для этого используем описание перехода изотропная жидкость — кристалл в рамках теории Ландау, в которой параметром порядка являются фурье-гармоники плотности $\rho_{\mathbf{G}}$ ^{2,3}. Хотя такой подход заведомо не годится для количественного описания процесса кристаллизации, можно надеяться, что качественные результаты, такие как пространственная симметрия упорядоченной фазы и знаки фурье-гармоник $\rho_{\mathbf{G}}$ окажутся правильными. Так как нас интересует структура низкотемпературной фазы, а не температура перехода, мы выберем свободную энергию F в простейшем виде

$$F = \frac{1}{V} \int d\mathbf{r} (-\rho^3 + \rho^4) = - \sum_{\mathbf{G}_1, \mathbf{G}_2} \rho_{\mathbf{G}_1} \rho_{\mathbf{G}_2} \rho_{-\mathbf{G}_1 - \mathbf{G}_2} + \sum_{\mathbf{G}_1, \mathbf{G}_2, \mathbf{G}_3} \rho_{\mathbf{G}_1} \rho_{\mathbf{G}_2} \rho_{\mathbf{G}_3} \rho_{-\mathbf{G}_1 - \mathbf{G}_2 - \mathbf{G}_3}, \quad (1)$$

где V — объем, а $\rho(\mathbf{r})$ — плотность кристалла. Рассмотрим функционал (1) для групп T^1-P23 и T^4-P2_13 , которые являются подгруппами всех остальных кубических групп. Ис-

$Pm3, Pa3, Im3, I2_13$

Аппроксимант MnSi, структура B20, пространственная группа $P2_13$

$x, x, x;$

$x_{\text{Si}} = 0.846$ (0.845)

$x_{\text{Mn}} = 0.138$ (0.155)

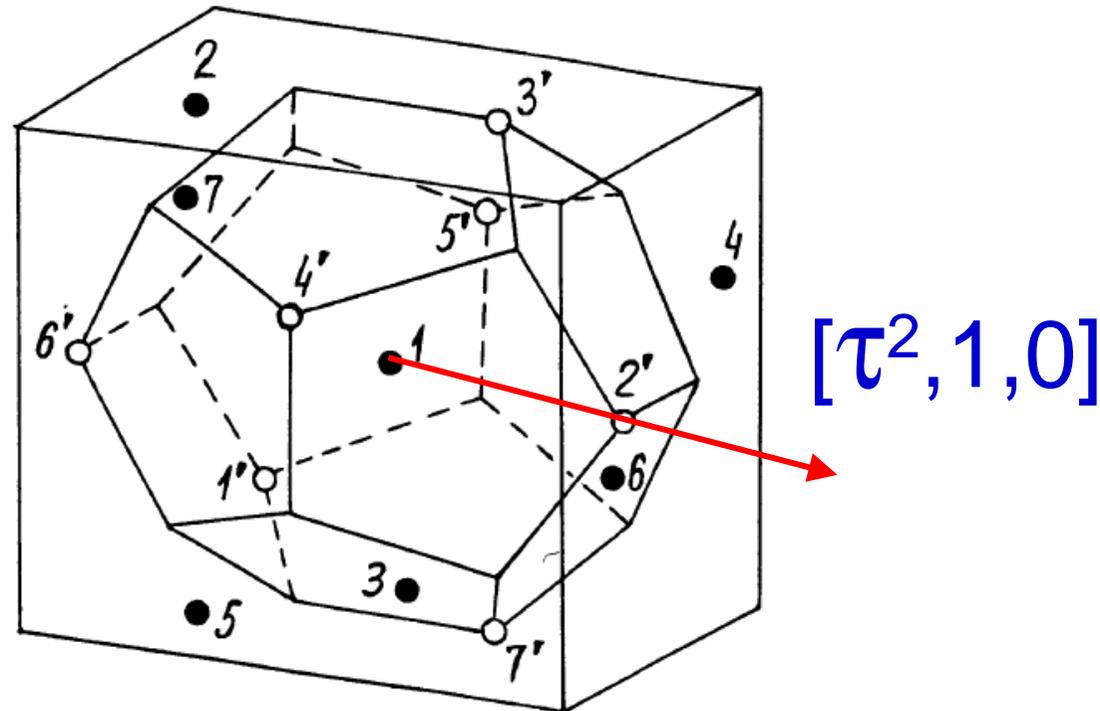
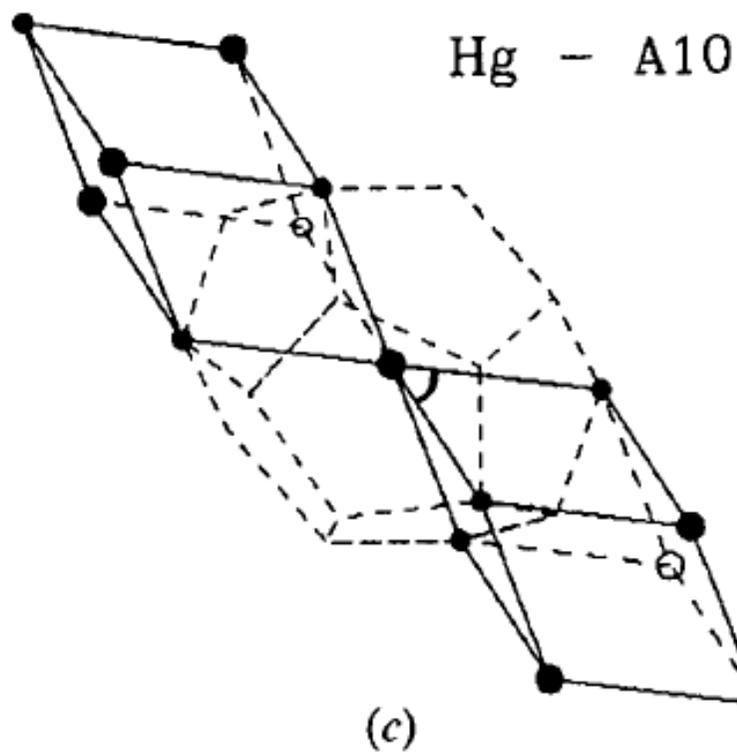
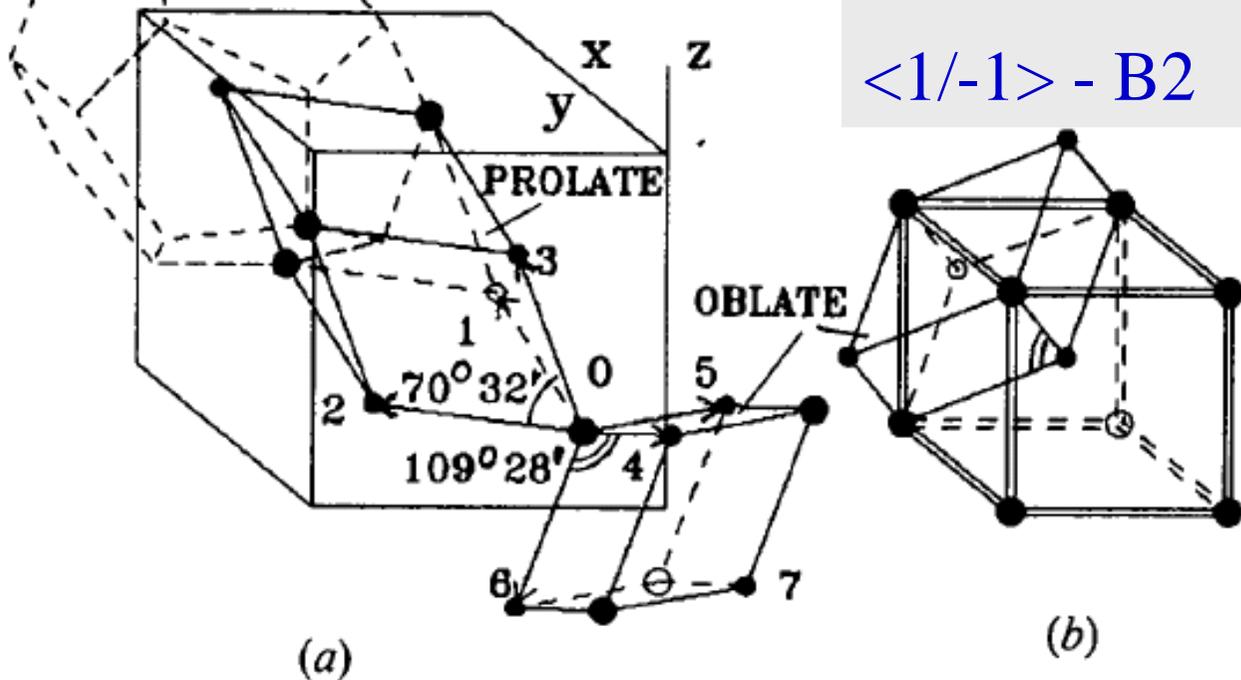


Fig. 6. — Idealized MnSi structure. Cube with the inscribed dodecahedron shows the unit-cell dimensions (conventional unit cell has another origin [20]). Full circles : A-atoms and empty circles : B-atoms. Atom 1 is at the center of the cube and atom 1' is at the cube diagonal ; the rest atoms are at the cube faces.

$\langle 0/1 \rangle$ - B20

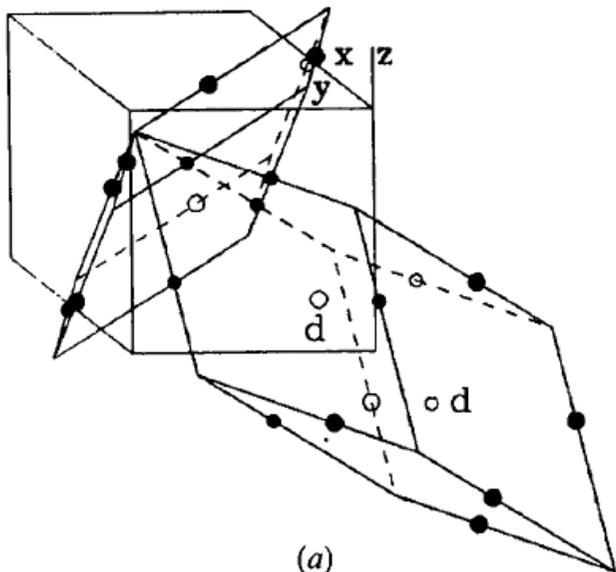
$\langle 1/-1 \rangle$ - B2

Додекаэдрическое
локальное
упорядочение в
простых
аппроксимантах



Декорированные ромбоэдры Амманна

$\langle 0/1 \rangle$ - B20



$\langle 0/1 \rangle$ - B20

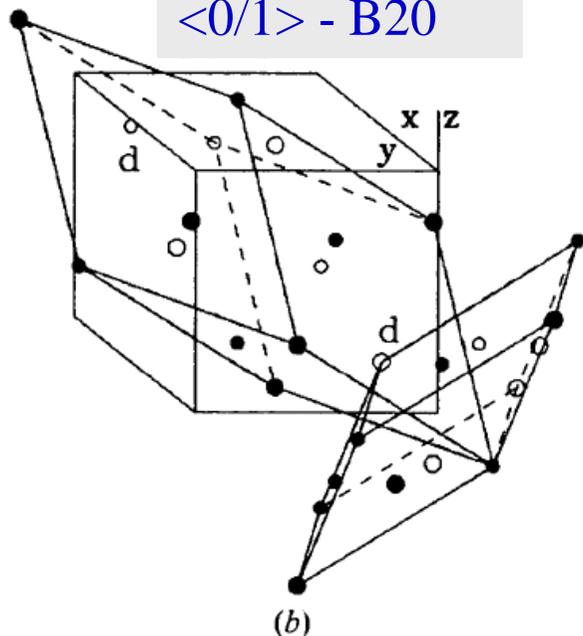


Fig. 3. Two different DLO-induced decorations of the Ammann rhombohedra in the same cubic approximant, $(2/1)_a$: (a) the edge decoration; (b) the vertex-face decoration. All the edges of the Ammann rhombohedra are directed along pseudo-fivefold axes. Large and small circles represent the *L* and *S* atoms, respectively; the letter *d* marks atoms at the body diagonals of the prolate Ammann rhombohedra. The cubes designate the unit cell of the B20 structure.

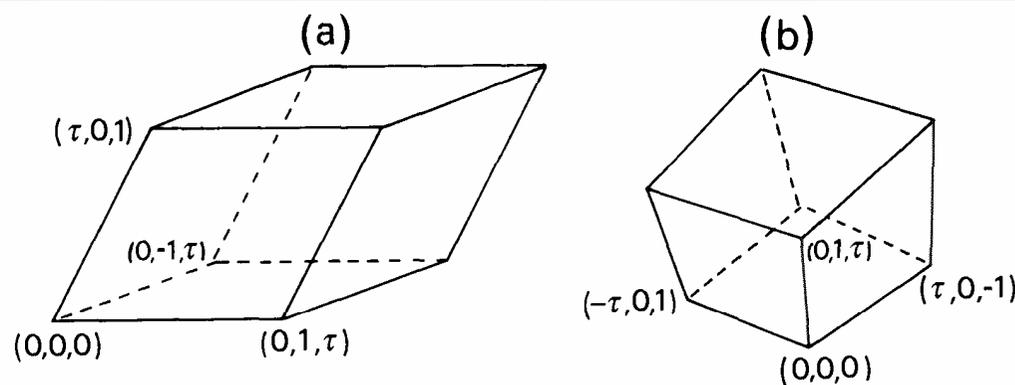


FIG. 1.23 Schematic of (a) prolate and (b) oblate rhombohedra that can be used for 3-dim Penrose tiling. Vertex coordinates are given in a frame of three orthogonal 2-fold axes of a regular icosahedron.

Малые и средние аппроксиманты

Table 1. *Positions of atoms and icosahedral holes in cubic approximants with DLO*

The hole marked by an asterisk is not icosahedral. Experimental values are given for the first compound of each approximant; for α -AlMnSi we take those positions that are less distorted by the atoms in the i -holes.

Label	Examples	Elser-Henley notations	Theoretical (x,y,z) coordinates in a unit cell	Experimental (x,y,z) coordinates in a unit cell	$(N'_b N_b N_c)$ or $(N'_a N_a)$	Six-dimensional indices
$\langle 1/1 \rangle$	FeSi	1/-1	(0,0,0)	(0,0,0)	(068)	000000
	AlPd		(0.5,0.5,0.5)	(0.5,0.5,0.5)	(068)	000111
$\langle 2/1 \rangle_a$	FeSi	0/1	(0.845,0.845,0.845)	(0.844,0.844,0.844)	(067)	111000
	AlPd		(0.155,0.155,0.155)	(0.136,0.136,0.136)	(067)	000000
$\langle 2/1 \rangle_b$	PdF ₂	0/1	(0.345,0.345,0.345)	(0.343,0.343,0.343)	(067)	000111
	FeS ₂		(0.655,0.655,0.655)	(0.657,0.657,0.657)	(067)	000000
	Pyrites		(0,0,0)	(0,0,0)	-	*hole
$\langle 3/2 \rangle$	Au ₃ NaSi	1/0	(0.095,0.095,0.095)	(0.097,0.097,0.097)	(067)	000000
	Au ₃ NaGe		(0.214,0.095,0.405)	(0.226,0.133,0.408)	(066)	001000
			(0.405,0.405,0.405)	(0.381,0.381,0.381)	(39)	i -hole
$\langle 5/3 \rangle_a$	Al ₅ Li ₃ Cu	1/1	(0.191,0.191,0.191)	(0.187,0.187,0.187)	(067)	000000
	Mg ₃₂ (AlZn) ₄₉		(0,0.118,0.191)	(0,0.094,0.154)	(075)	010000
	Au ₄ Na ₃ Si ₂		(0,0.309,0.118)	(0,0.305,0.117)	(076)	010100
	Au ₃ Na ₂ Sn		(0.118,0.191,0.382)	(0.157,0.190,0.406)	(066)	000001
			(0.427,0,0.5)	(0.404,0,0.5)	(156)	110012
			(0.191,0,0.5)	(0.199,0,0.5)	(058)	101001
			(0.191,0.309,0)	(0.175,0.301,0)	(39)	i -hole
(0,0,0)	(0,0,0)	(0,12)	i -hole			
$\langle 5/3 \rangle_b$	α -AlMnSi	1/1	(0.118,0.191,0.309)	(0.115,0.187,0.300)	(076)	000000
	α -AlFeSi		(0.5,0.191,0.309)	(0.5,0.180,0.308)	(067)	100100
	Sc ₅₇ Rh ₁₃		(0.5,0.118,0.118)	(0.5,0.120,0.117)	(065)	101100
	Hf ₅₄ Os ₁₇		(0.118,0.118,0.118)	(0.164,0.100,0)	(067)	001000
			(0.5,0.5,0.118)	(0.5,0.5,0.122)	(156)	111110
			(0,0,0.236)	?	(156)	100010
			(0,0,0)	?	(068)	001111
	(0.309,0,0.5)		(0.290,0,0.5)	(2,10)	i -hole	

Аппроксиманты Фибоначчи: от малых к большим

1/0: A.A.A.A.A.A.A.A подстановка: $A \rightarrow AB$, $B \rightarrow A$

1/1: AB.AB.AB.AB.AB.AB.AB.AB.AB

2/1: **ABA.ABA.ABA.ABA.ABA.ABA.ABA**

3/2: **ABAAB.ABAAB.ABAAB.ABAAB.ABAAB**

5/3: ABAABABA.ABAABABA.ABAABABA

8/3: ABAABABAABAAB.ABAABABAABAAB.

Approximants 2/1: Al-Pd-Mn-Si [1], Al-Rh-Si [2,3], Al-Mg-Zn [4], and Ca-Cd [5]

- the structure is idealized: 5-, 3-, 2-fold bonds
- **all the atoms** are lifted to a 6-dim cubic lattice and then projected to the perpendicular space
- the deviations from the ideal positions in the physical space are analyzed

[1]. K. Sugiyama, N. Kaji, K. Hiraga, T. Ishimasa, Z. Kristallogr. 1998. **213**. 90.

[2]. K. Sugiyama, W. Sun, K. Hiraga. J. Non-Cryst. Solids. 2004. **334&335**. 156.

[3]. T. Takeuchi, N. Koshikawa, E. Abe, K. Kato, U. Mizutani. J. Non-Cryst. Solids. 2004. **334&335**. 161.

[4]. Q. Lin, J.D. Corbett. Proc. Nat. Acad. Sci. 2006. **103**. 13589.

[5]. C.P. Gomez, S. Lidin. Angew. Chem. Int. Ed. 2001. **40**. 4037.

The positions in the perp space and the deviations are listed in Crystallography Reports, 2007.

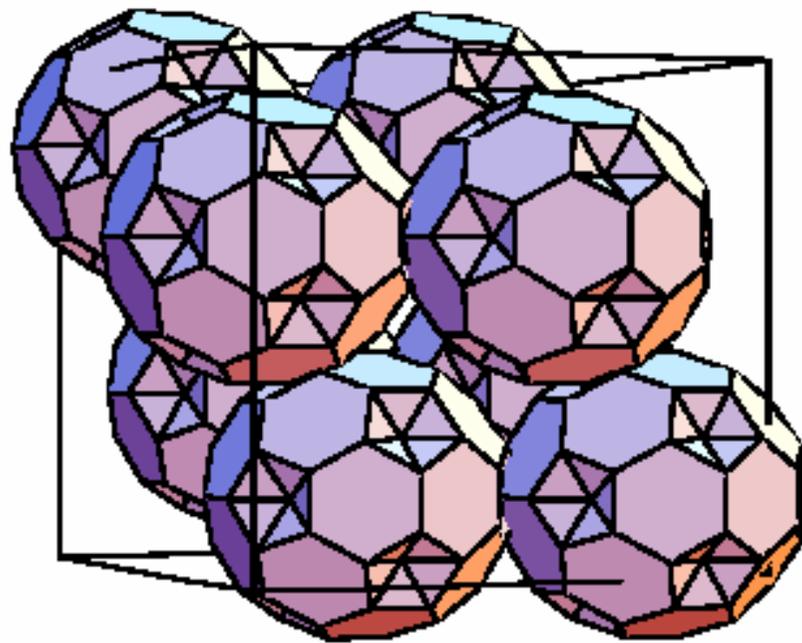
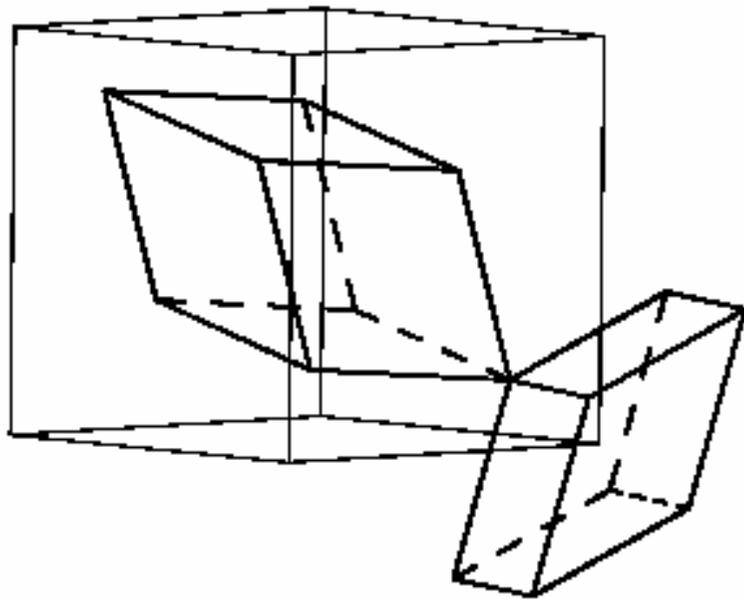


Fig. 1: Each unit cell of the 2/1-approximant contains eight Bergman clusters.

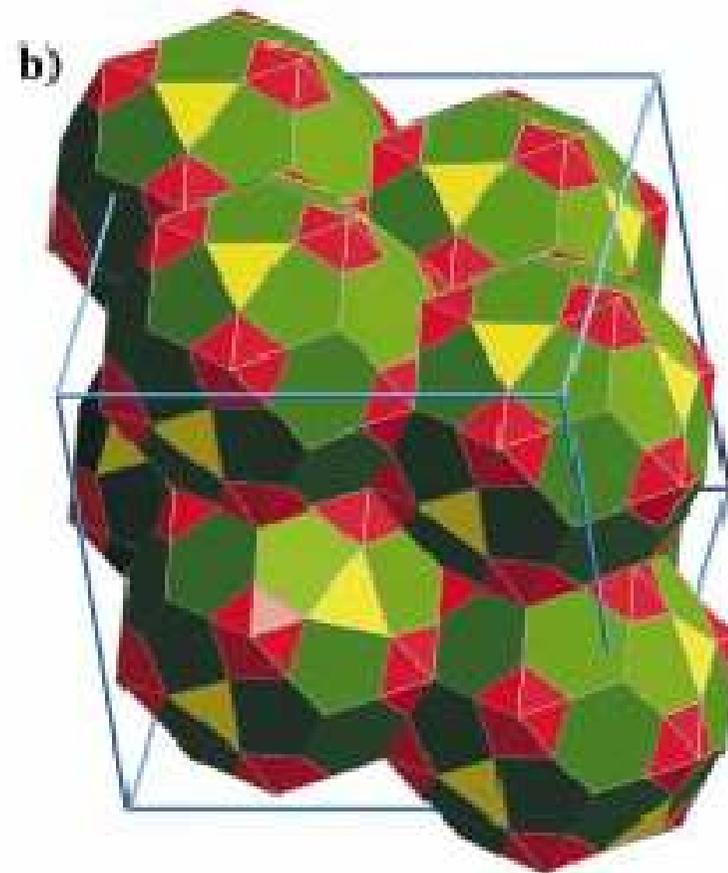


Al-Mg-Zn, $Pa\bar{3}$ space group,
about 704 atoms

S. Spiekermann, G. Kreiner, 1998

Ca-Cd, $Pa\bar{3}$ space group,
about 712 atoms

C.P. Gomez, S. Lidin, 2001



Al-Rh-Si, $Pm\bar{3}$, about 563 atoms

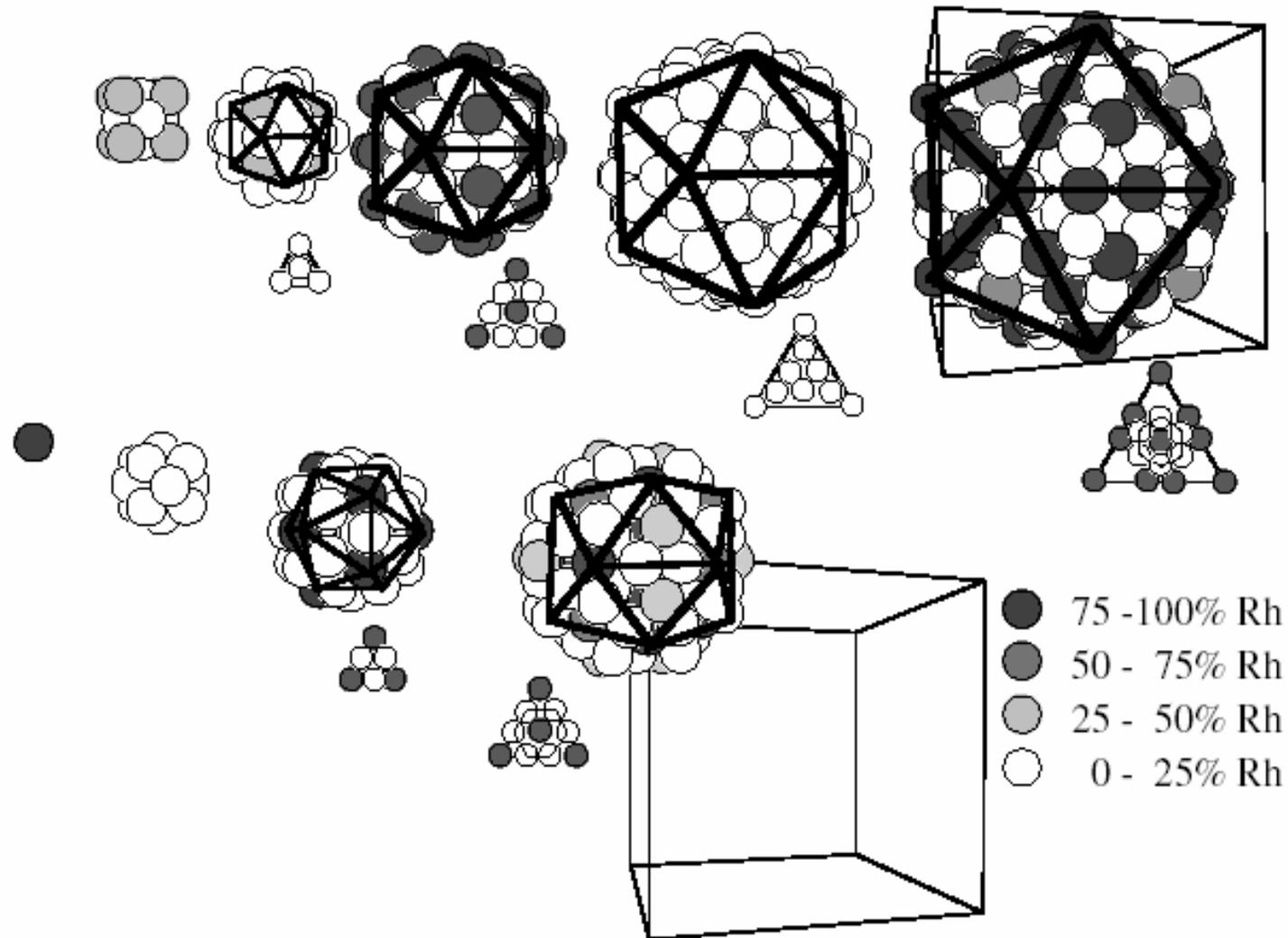
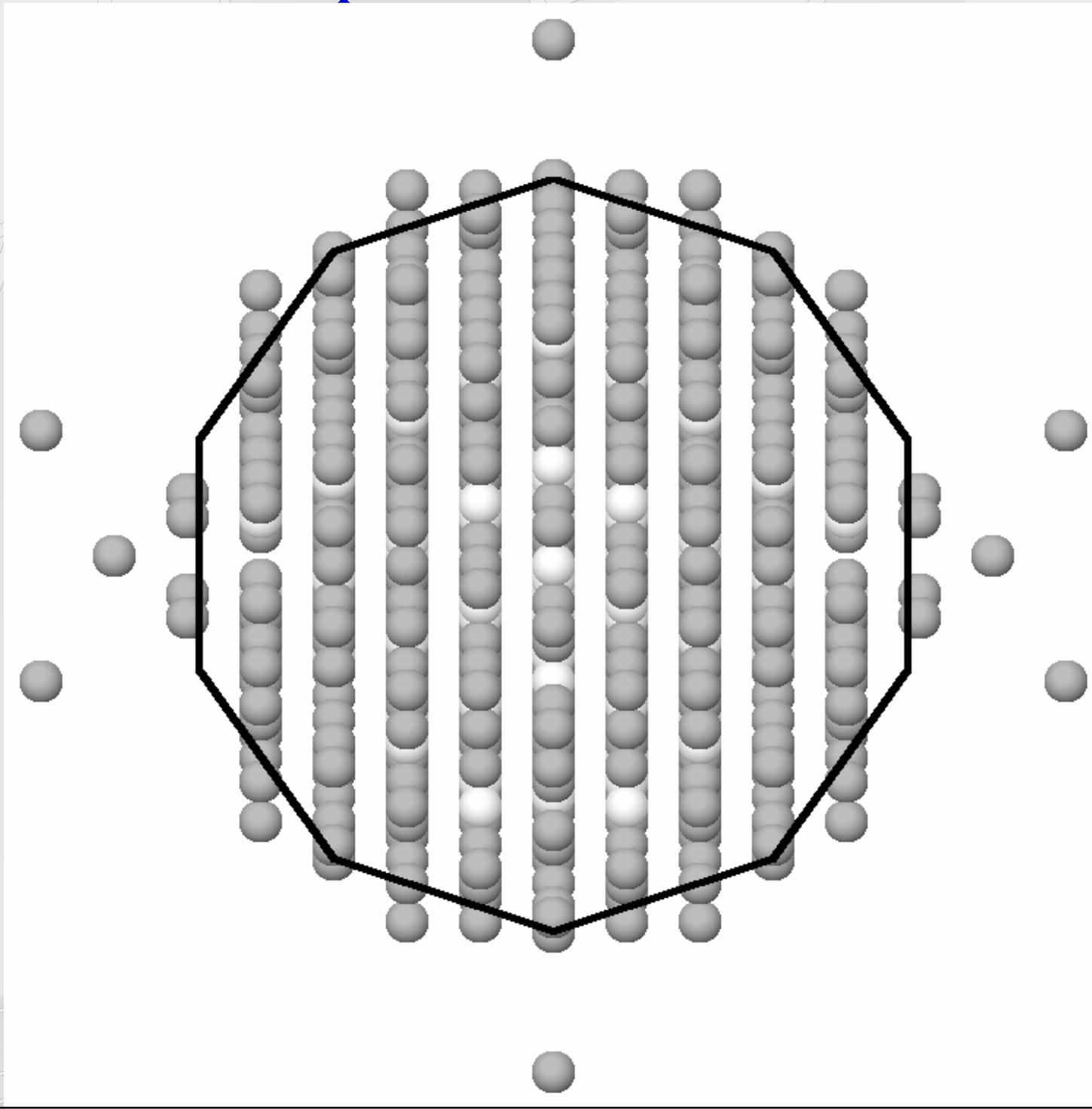
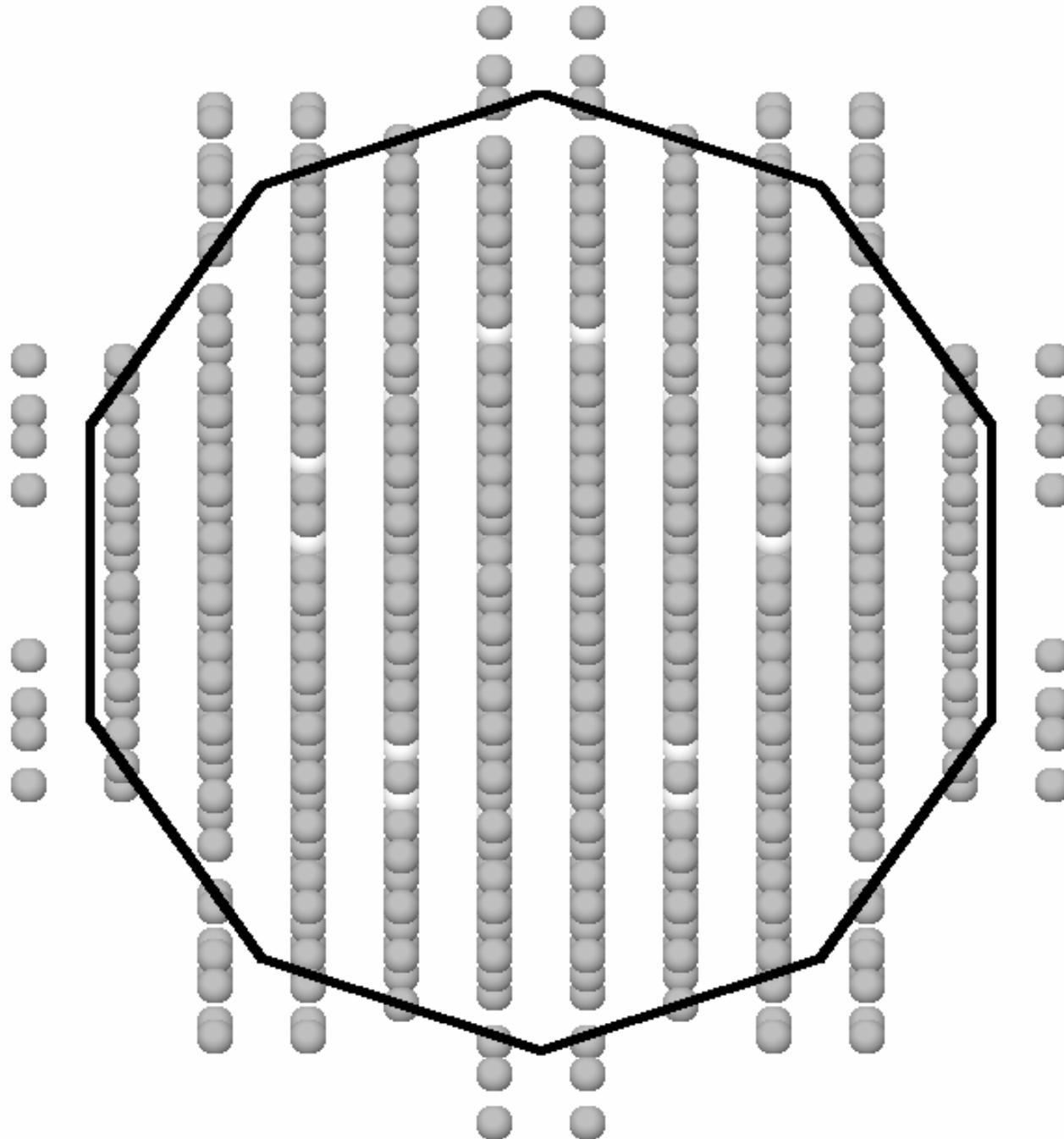


Fig. 4. Atomic clusters exist at the body center (top panel) and vertices (bottom panel) in the unit cell of the $Al_{65}Rh_{27}Si_8$ $2/1-2/1-2/1$ approximant. Atomic arrangements on the triangular faces of each icosahedral atomic shell are shown below each atomic shell. Open circles and filled circles indicate (Al, Si) and Rh atoms, respectively. The atomic sites in which Al and Re coexist together are expressed as gray circles. The depth of the gray color indicates the Re occupancy in each mixed site; the darker the color is, the more the Re exist. The triangles decorated by circles indicate the atom arrangements on the triangular faces of the icosahedral cluster shells. Note that the seven atoms on the faces along the $[1\ 1\ 1]$ direction in the fifth shell of the larger cluster centered at the body center are shared by the third shell in the small cluster centered at the vertices. Seven atoms constructing hexagons in the triangular surfaces of the outermost shells in the large cluster at body center of the unit cell are shared with the outermost shells in the small icosahedral clusters at vertices.

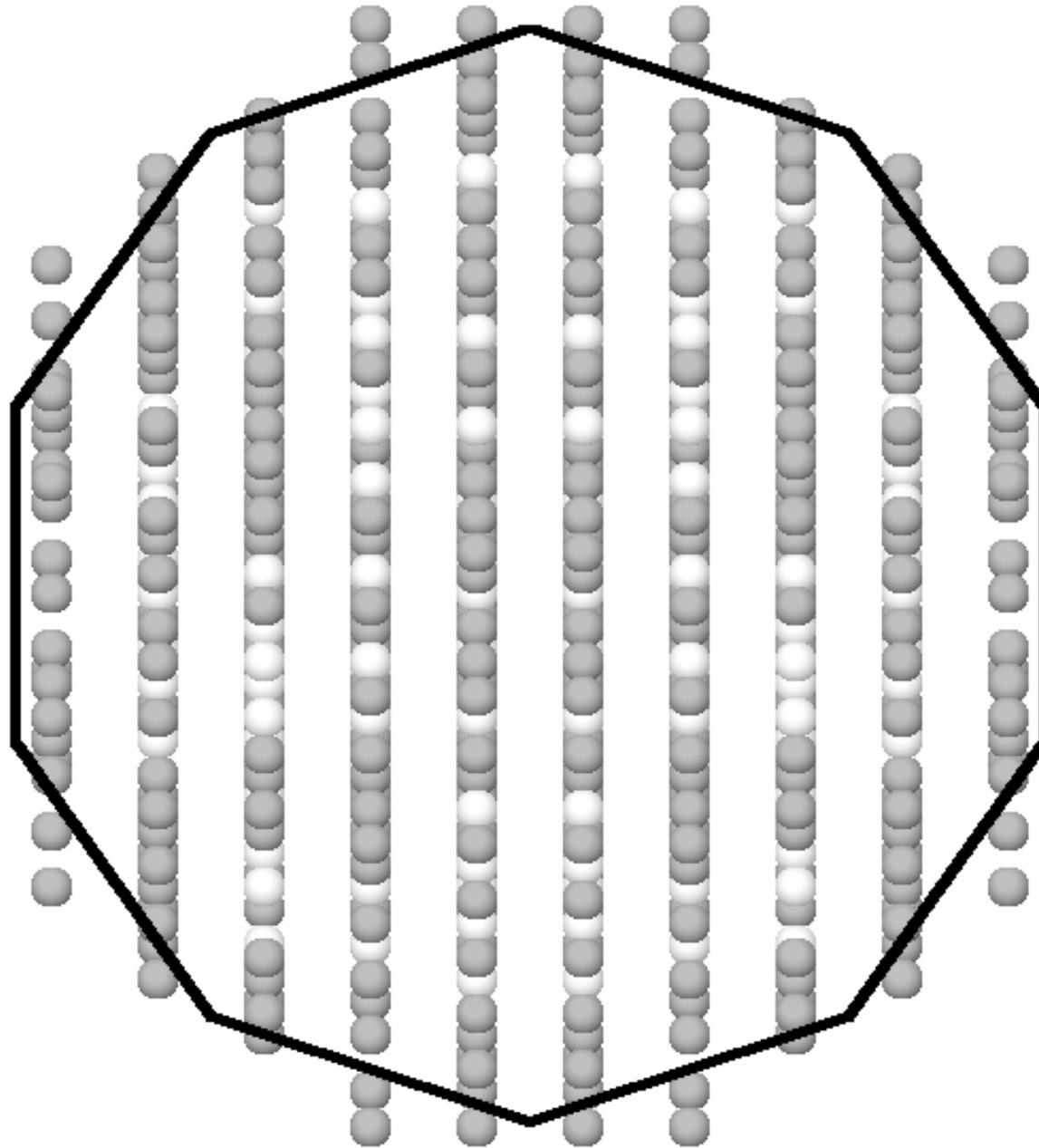
Perp view: Al-Rh-Si



Perp view: Ca-Cd



Perp view: Al-Mg-Zn



Метастабильная фаза ВС8 в кремнии

Пространственная группа симметрии $Ia\bar{3}$, 16 атомов на ячейку

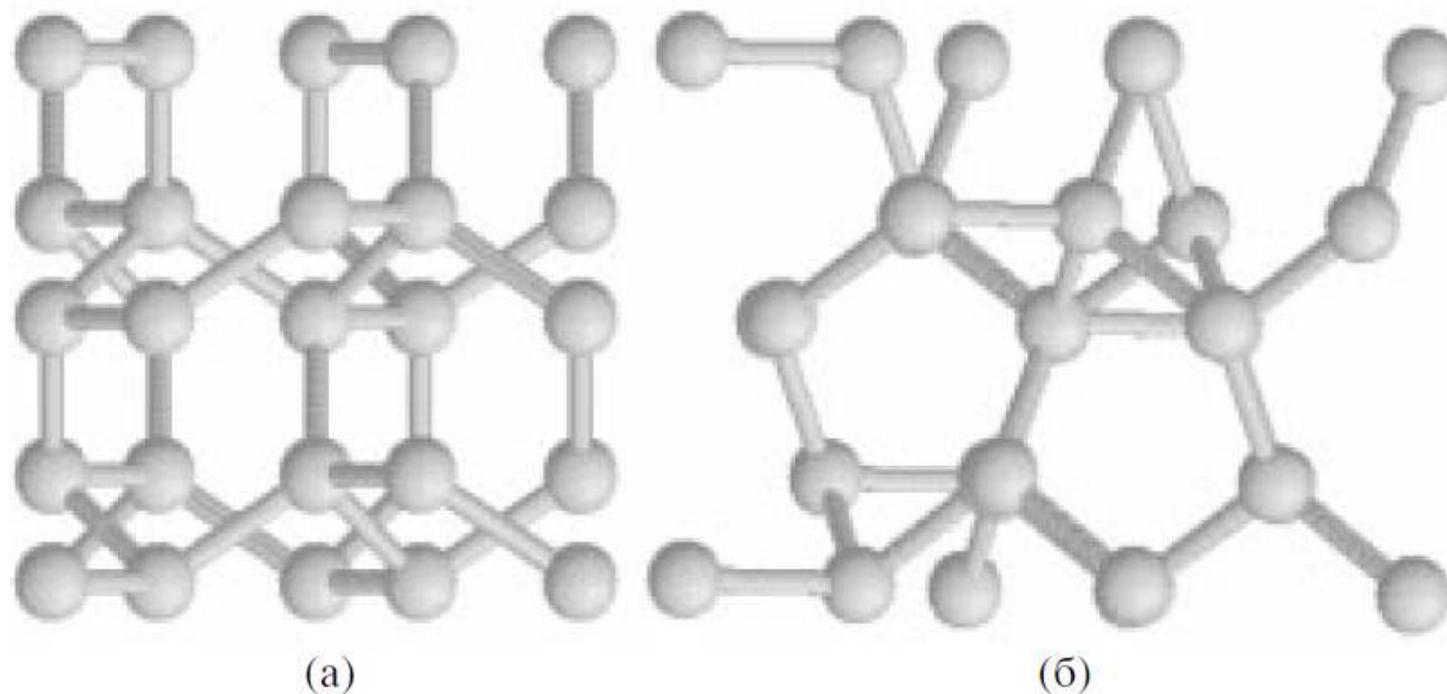


Рис. 2. Вид на структуру ВС8: а – вдоль оси z , б – вдоль оси пятого порядка. Показаны атомы и связи. Видны правильные пятиугольники и половинка десятиугольника (б), однако следует подчеркнуть, что эти фигуры не плоские.

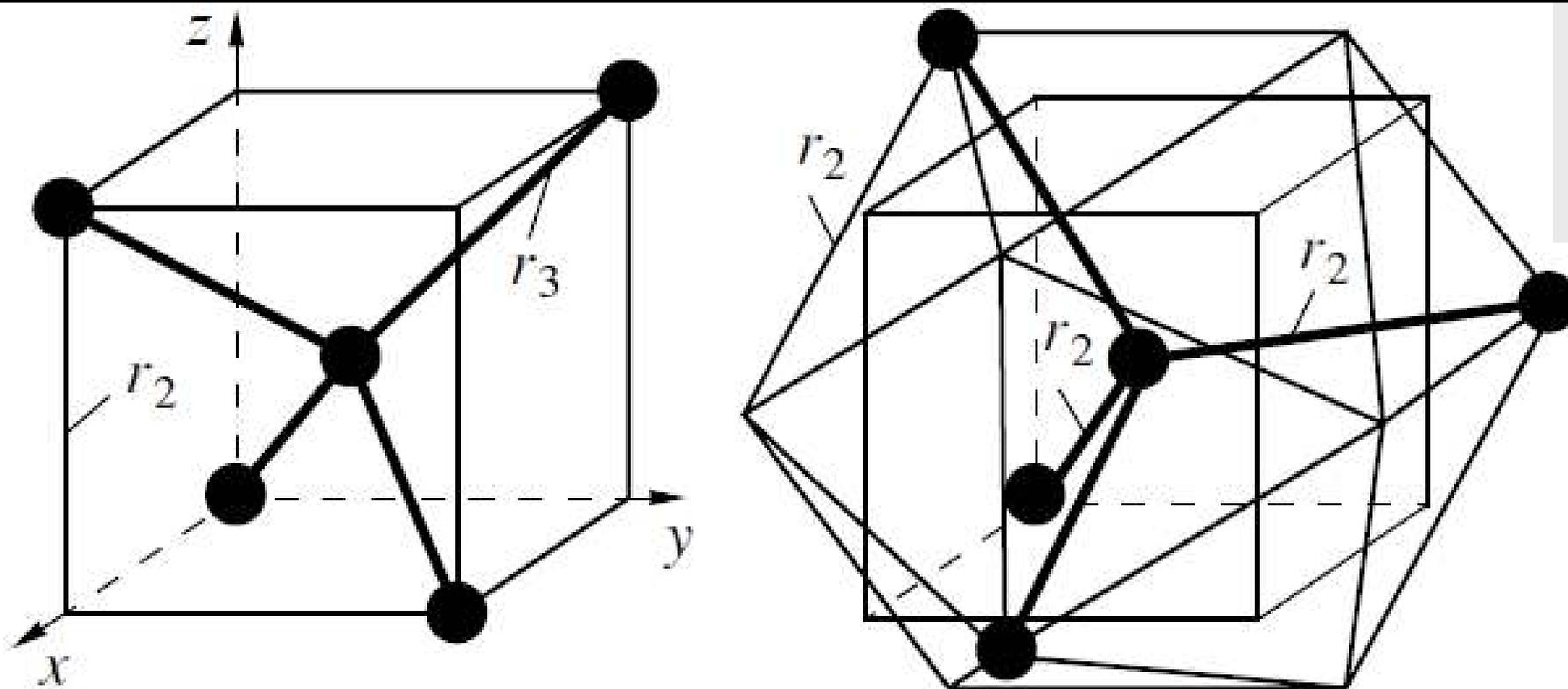


Рис. 1. Тетраэдрическое упорядочение в структуре алмаза (а) и в фазе BC8 (б). Ковалентные связи показаны жирными линиями. В идеальной структуре ребра икосаэдра в точности равны ребрам кубов (невидимые ребра икосаэдра не показаны для простоты). Кубы на рисунках (а) и (б) одинаковы, их ребра в 2 раза меньше постоянной решетки структуры алмаза или в τ^2 раз меньше постоянной решетки фазы BC8. В обоих случаях центр инверсии находится в середине связи, направленной вдоль оси третьего порядка.

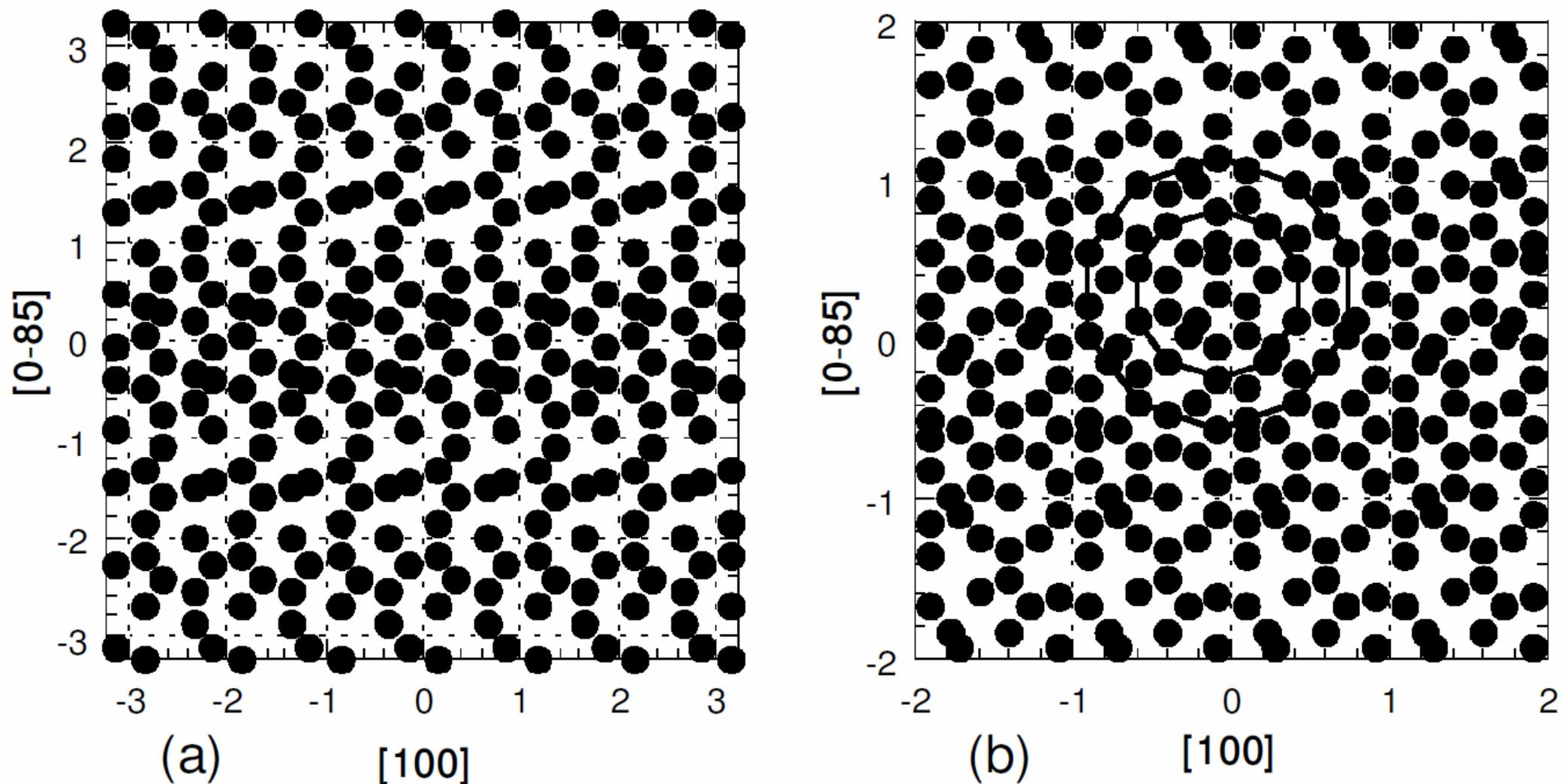


Figure 1. Pentagonal and decagonal motifs in the BC8 phase, which is the $1/0$ approximant, (a) and in the $1/1$ approximant (b). Atomic layers normal to the $[058]$ direction are shown. All distances are given in unit cell sizes which are different by τ . Two complete τ -scaled decagons are indicated by solid lines.

Фазонные прыжки атомов

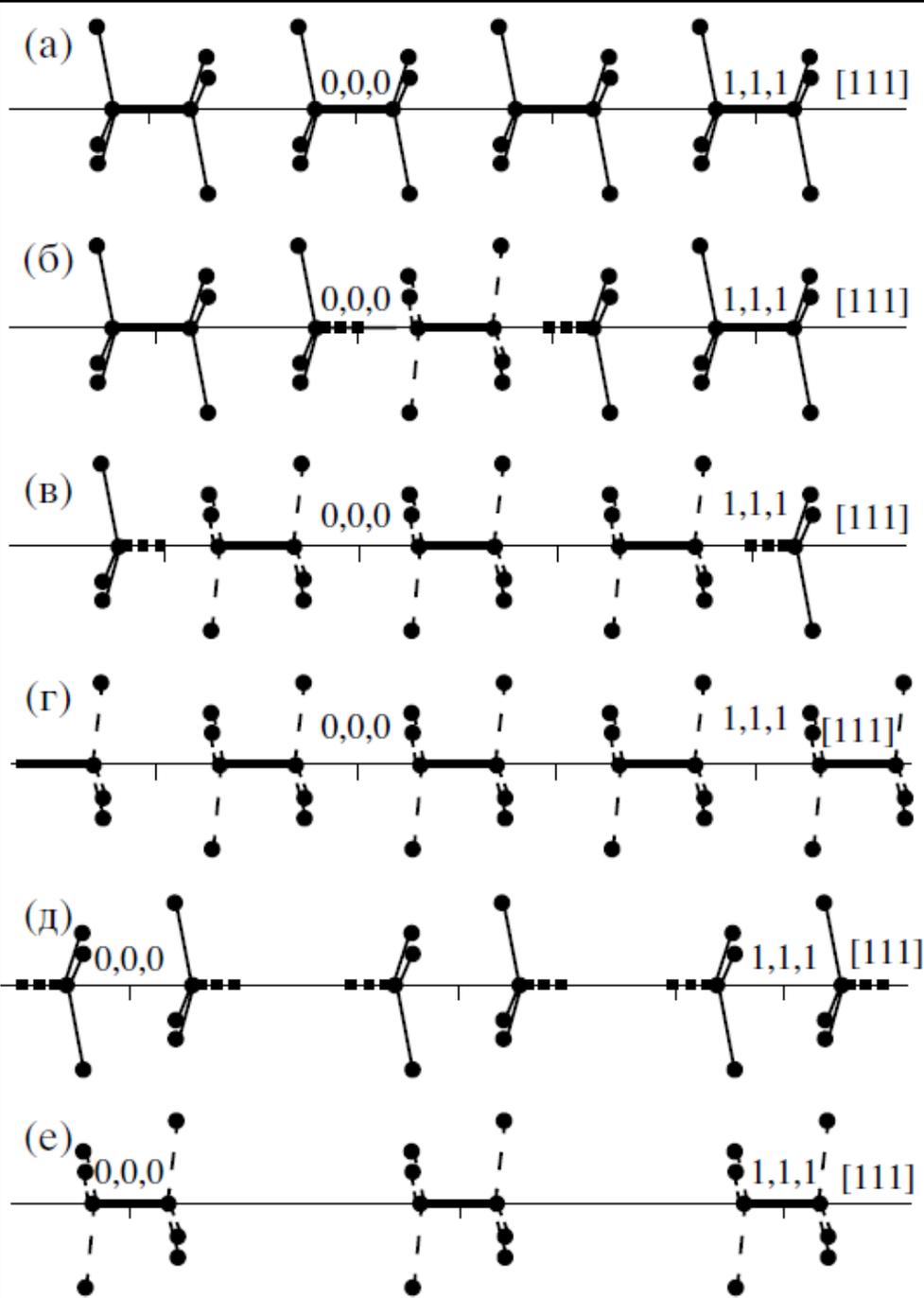
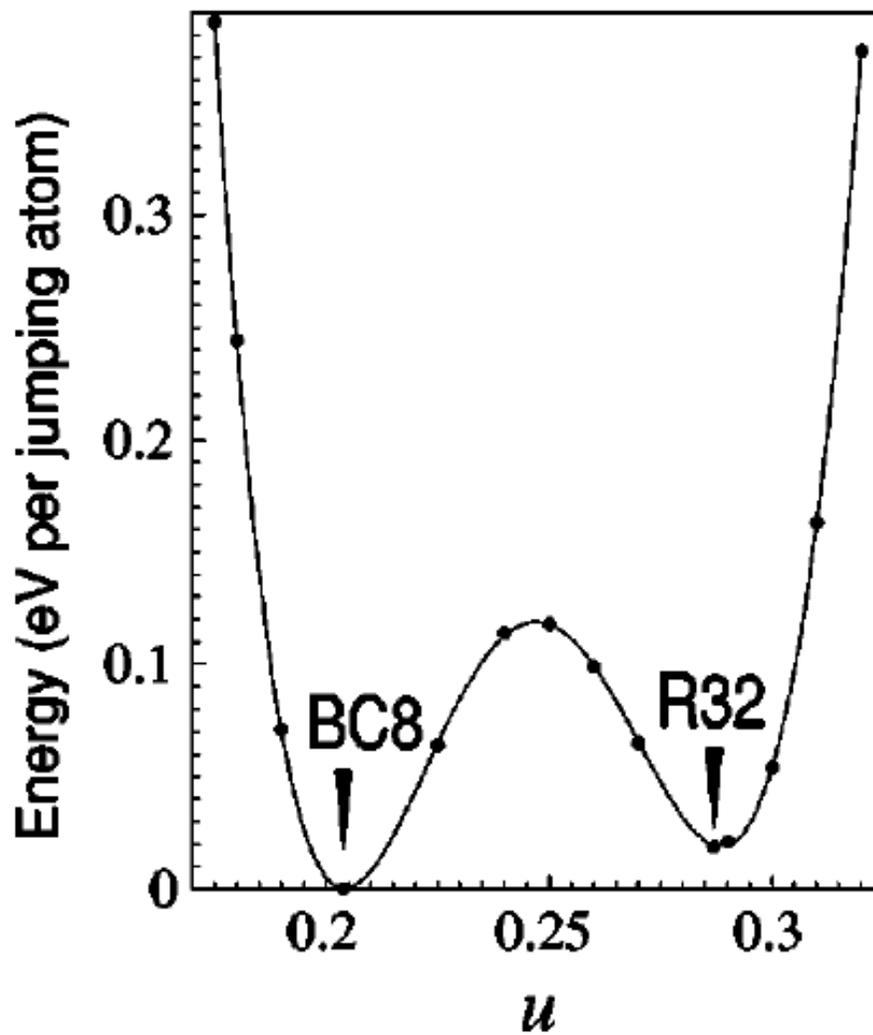


Рис. 3. Образование фазонных дефектов в аппроксимантах 1/0 (фаза VC8) и 1/1. А-связи – жирные линии, В-связи – сплошные линии, С-связи – штриховые линии, оборванные связи – жирные штриховые линии.



Энергия
 фазонных
 прыжков
ab initio

PARATEC
 DFT+LDA

FIG. 7. Energetics of an isolated phason flip. Energy of two jumping atoms (relative to the perfect BC8 phase) is given as a function of their position u . Parameter u is given for the primitive rhombohedral supercell containing 32 atoms (for the BC8 cubic unit cell it would be twice smaller).

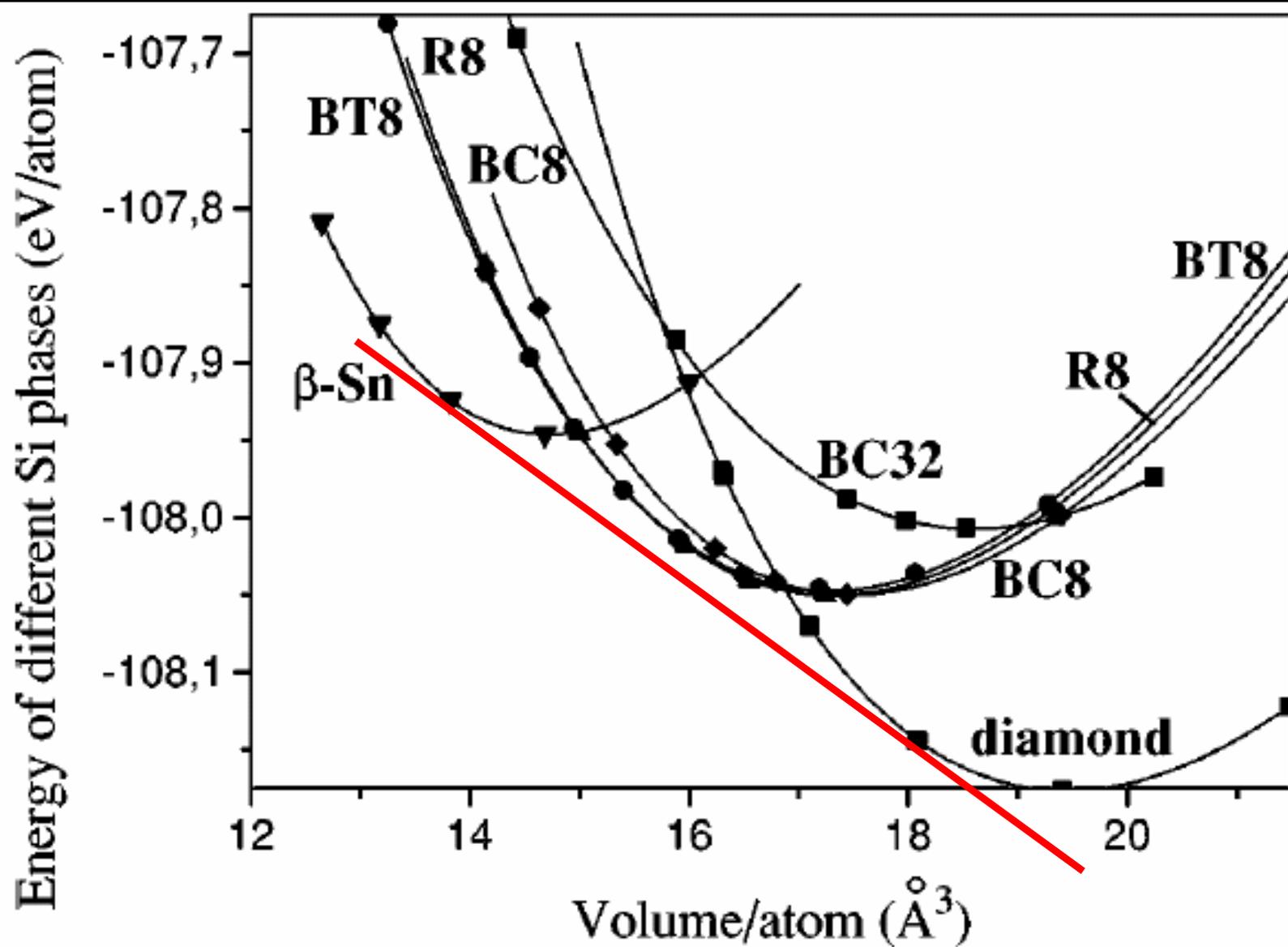


FIG. 3. Calculated energy of different Si phases as a function of volume per atom. Energies of BC8, R8, and BT8 phases are rather close for any density. The BC32 phase has larger energy and little chance to exist even as a metastable phase. Lines shows the Mur-naghan fit of the points.

Связь с аморфными структурами

Icosahedral order and disorder in semiconductors

365

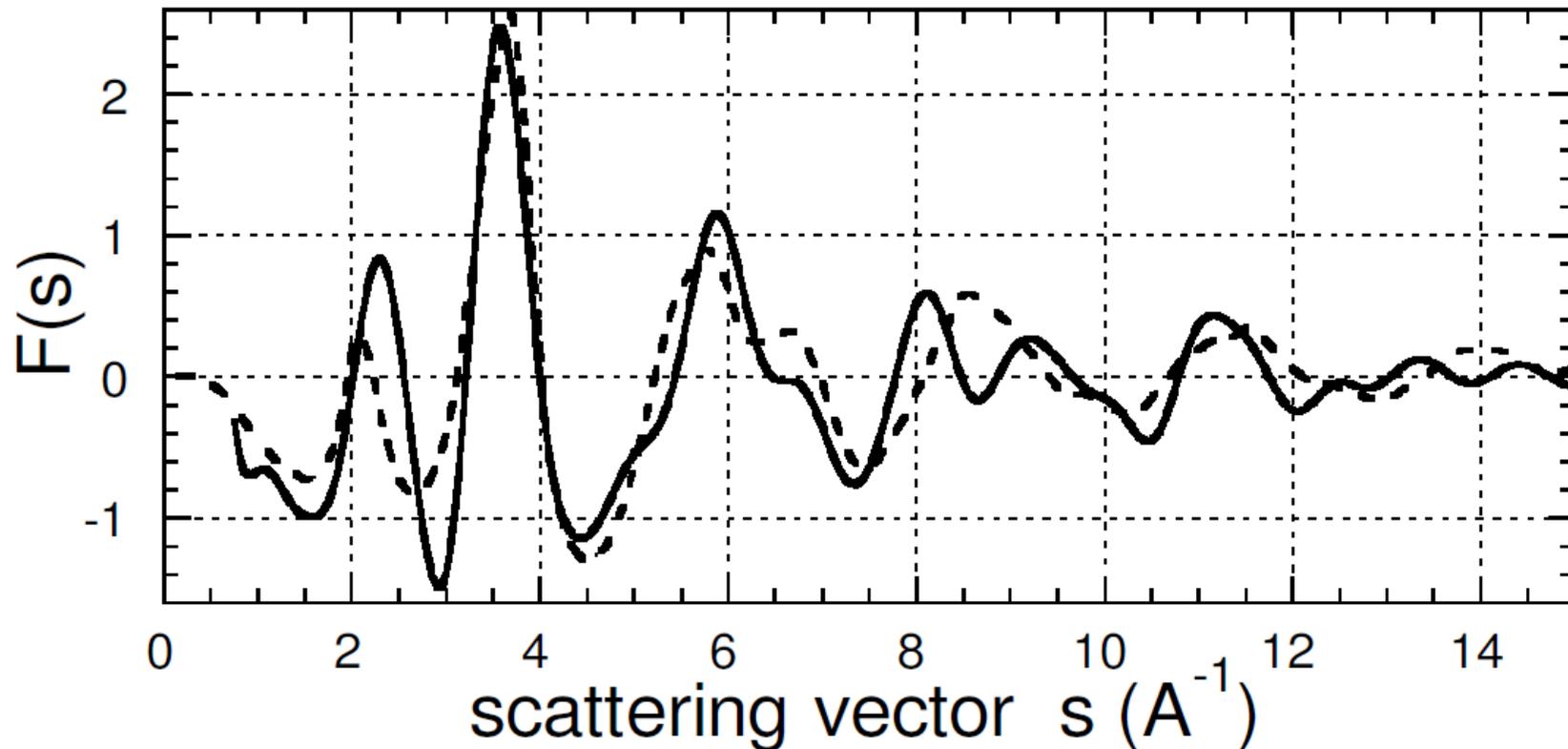


Figure 3. Reduced intensity function, $F(s)$, for the disordered BC8 phase (solid line) and for amorphous Si (dashed line), (Moss and Graczyk (1969), with permission).

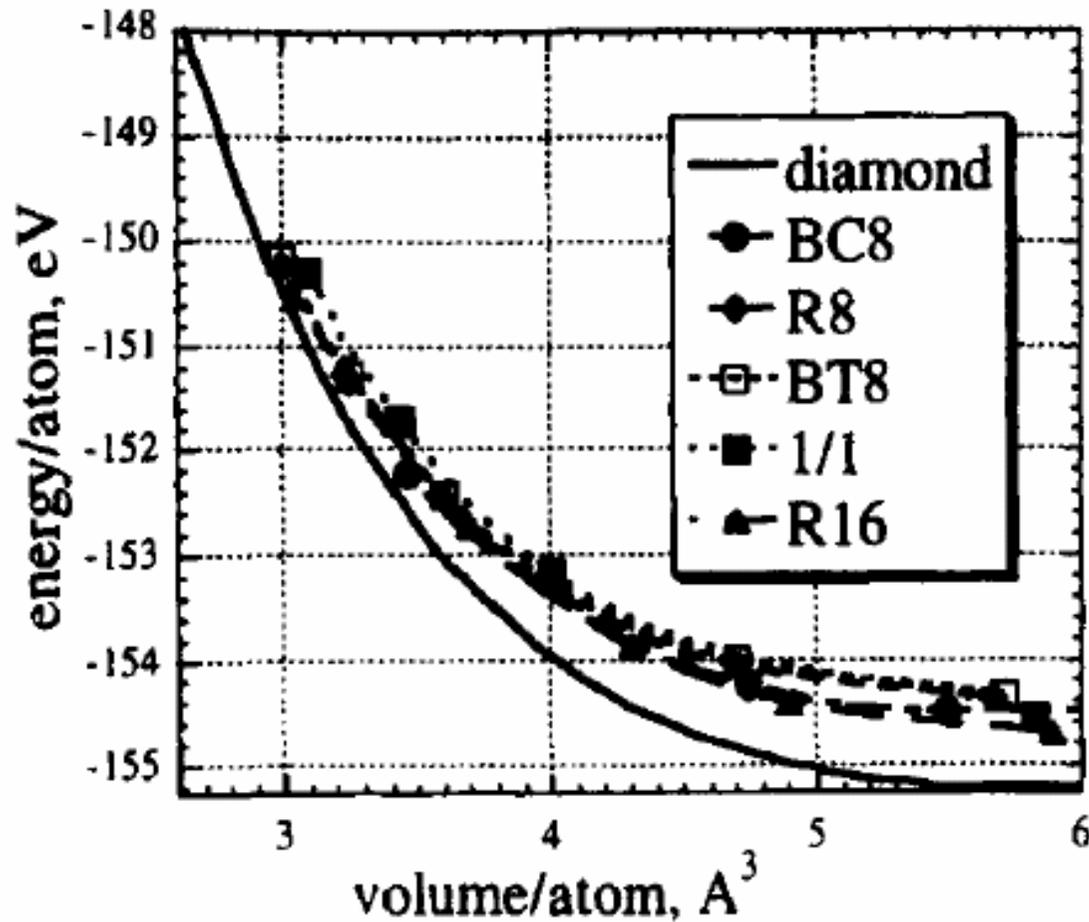
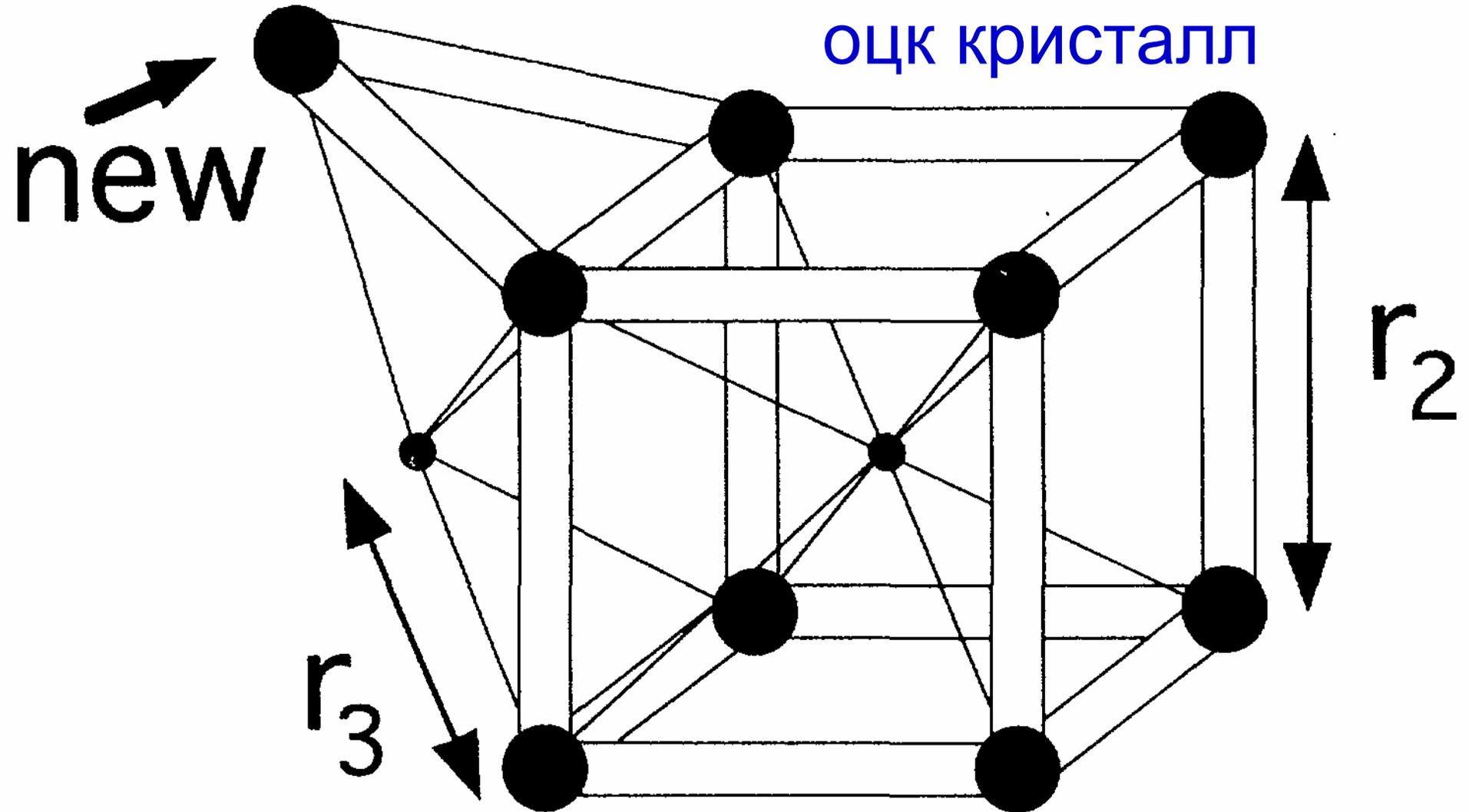
Энергии фаз
углерода

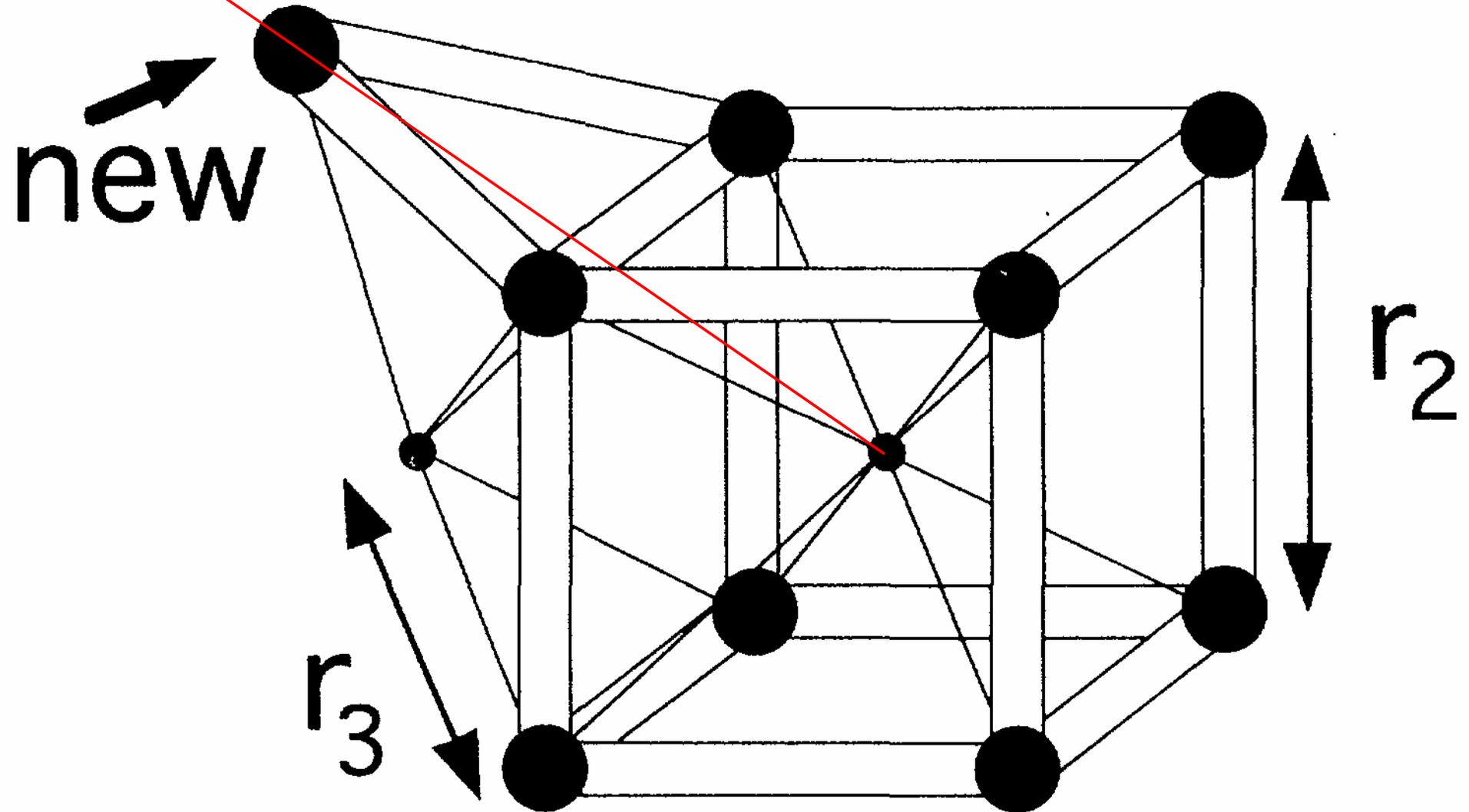
Figure 1: Calculated energy of four-coordinated carbon phases as a function of volume per atom (for $3 \text{ \AA}^3/\text{atom}$ the pressure is approximately 800 GPa). Energies of all quasicrystal-related phases are rather close to each other for any density and slightly higher than that of diamond.

От кубика до икосаэдра

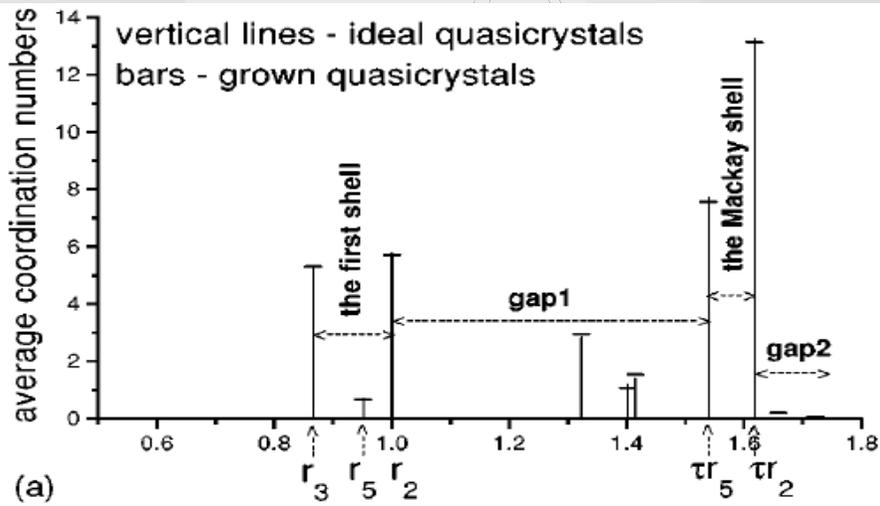


От кубика до икосаэдра

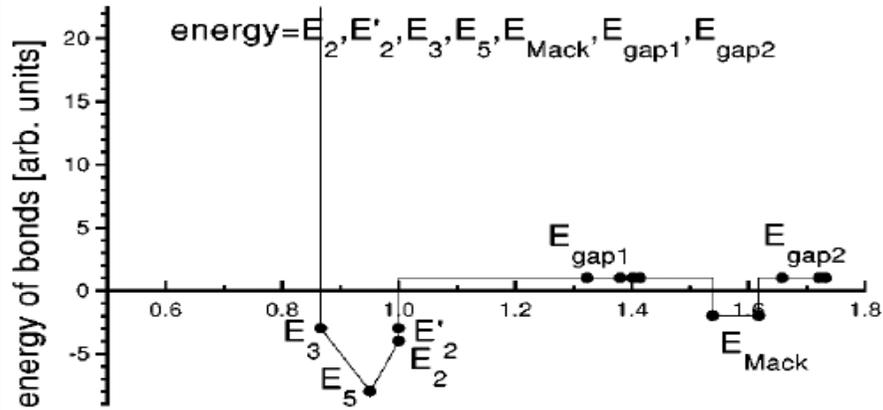
5-fold, $[\tau, 1, 0]$



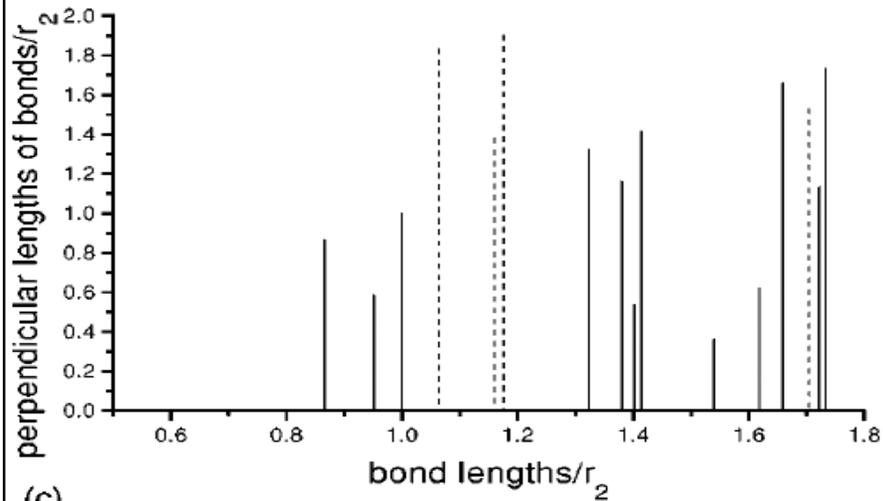
Как подавить рост кристалла?



(a)



(b)



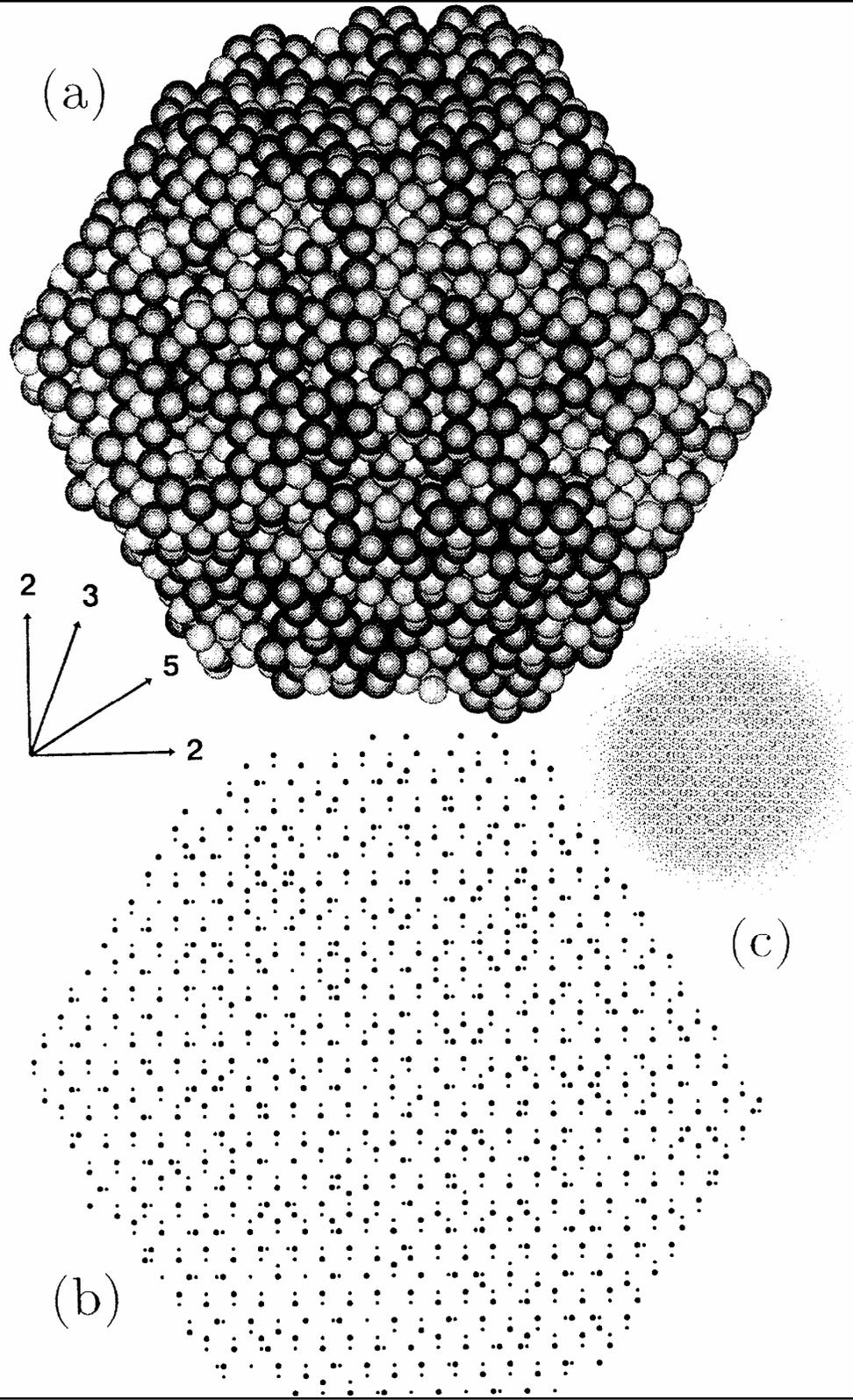
(c)

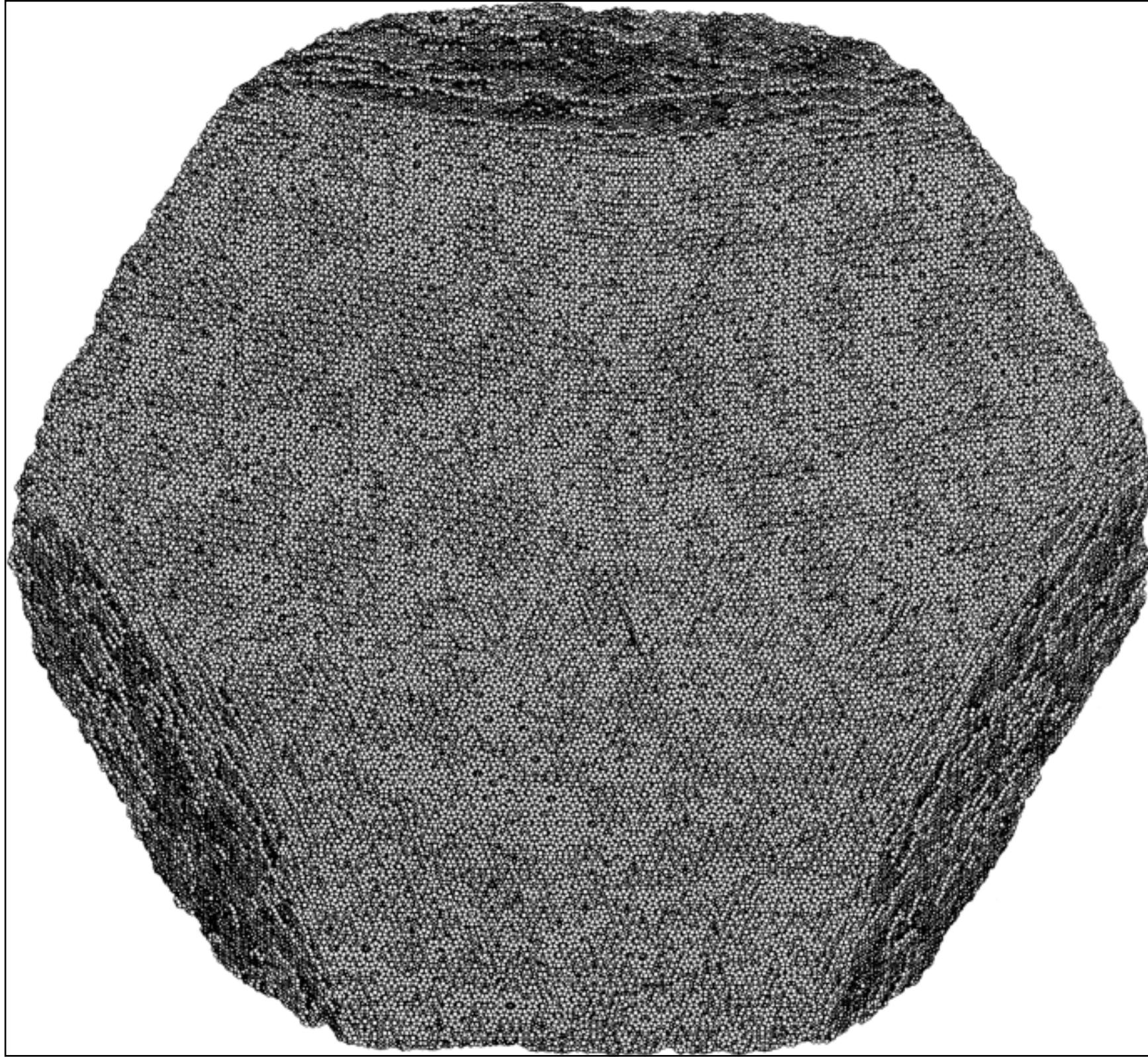
← координационные сферы в квазикристалле

← потенциал взаимодействия

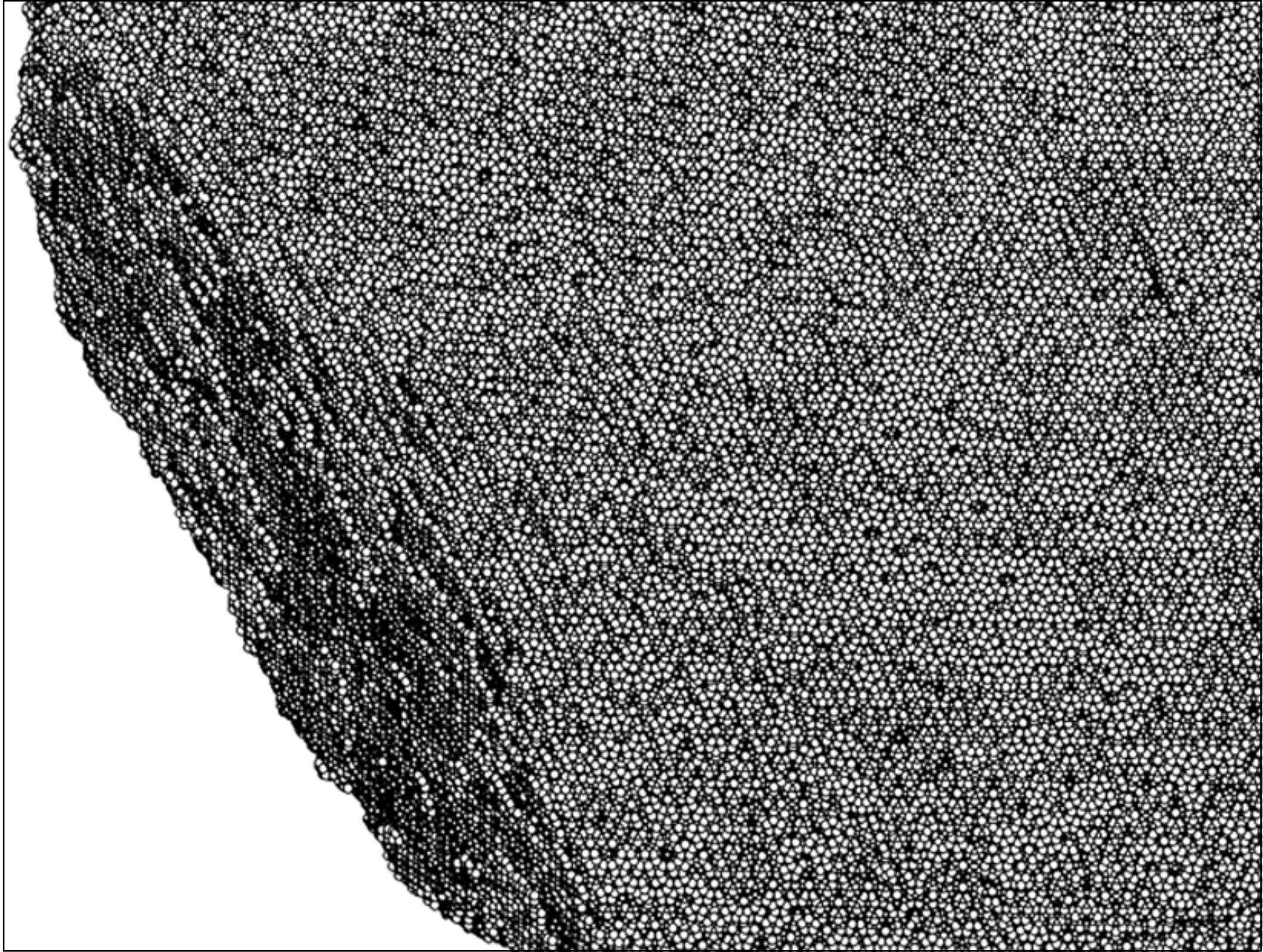
← расстояния в перпендикулярном пространстве

Начало роста, видна огранка
плоскостями \perp осям 5

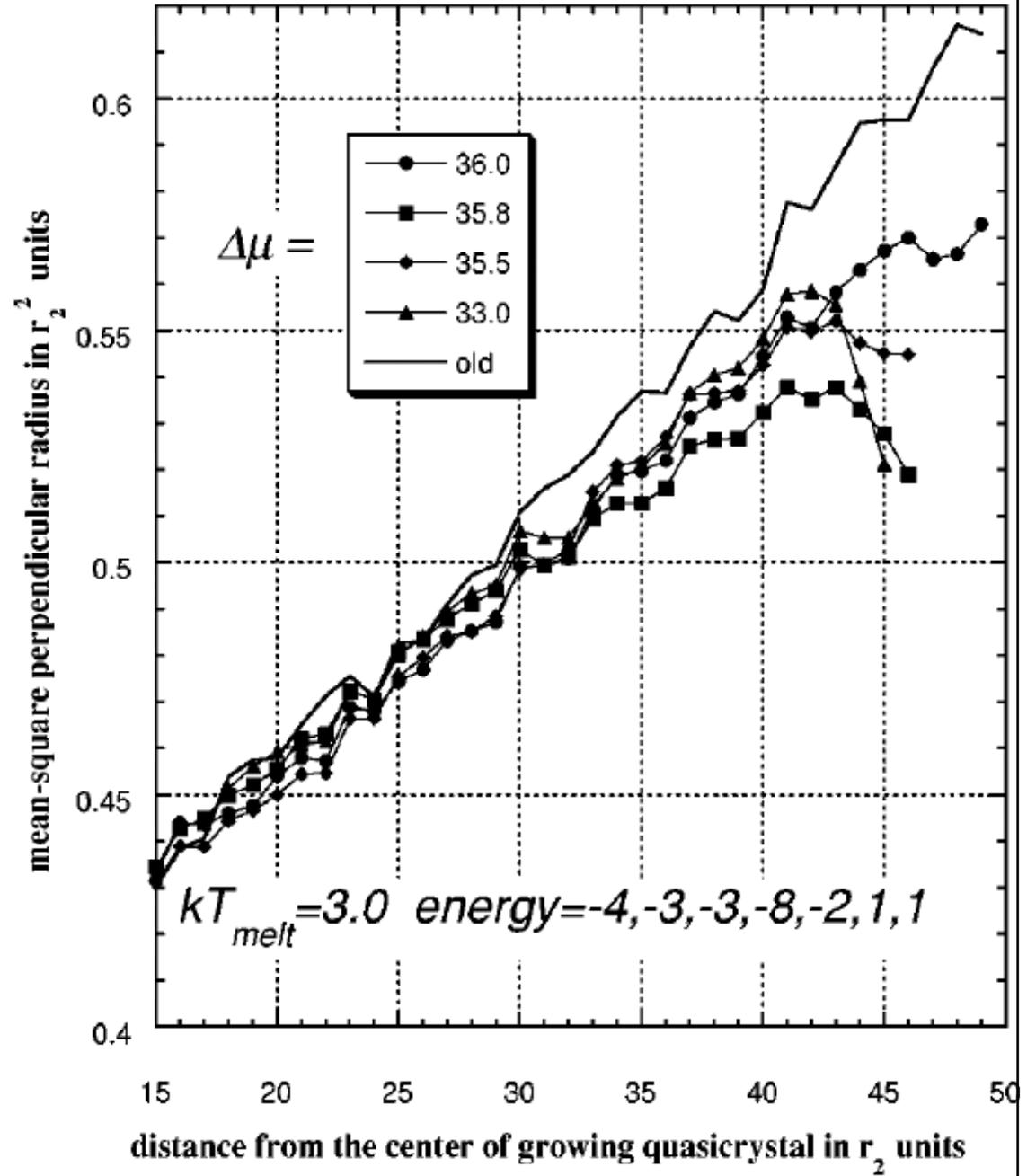
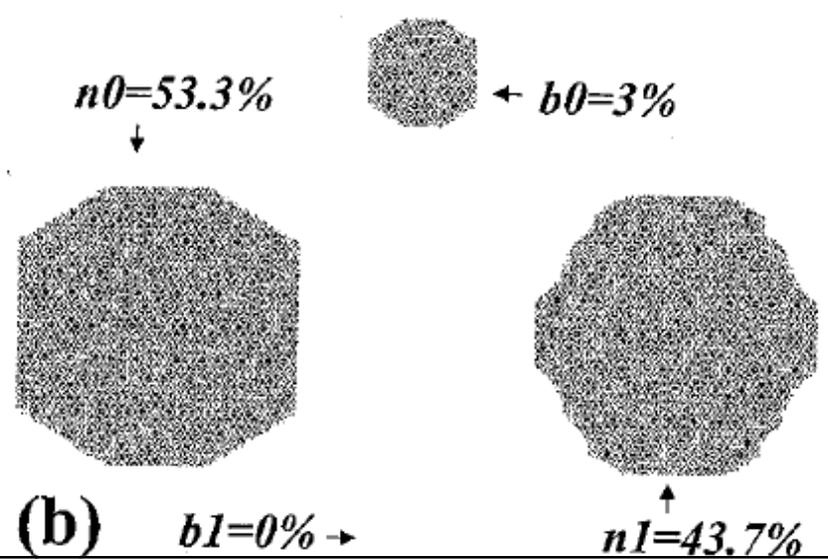
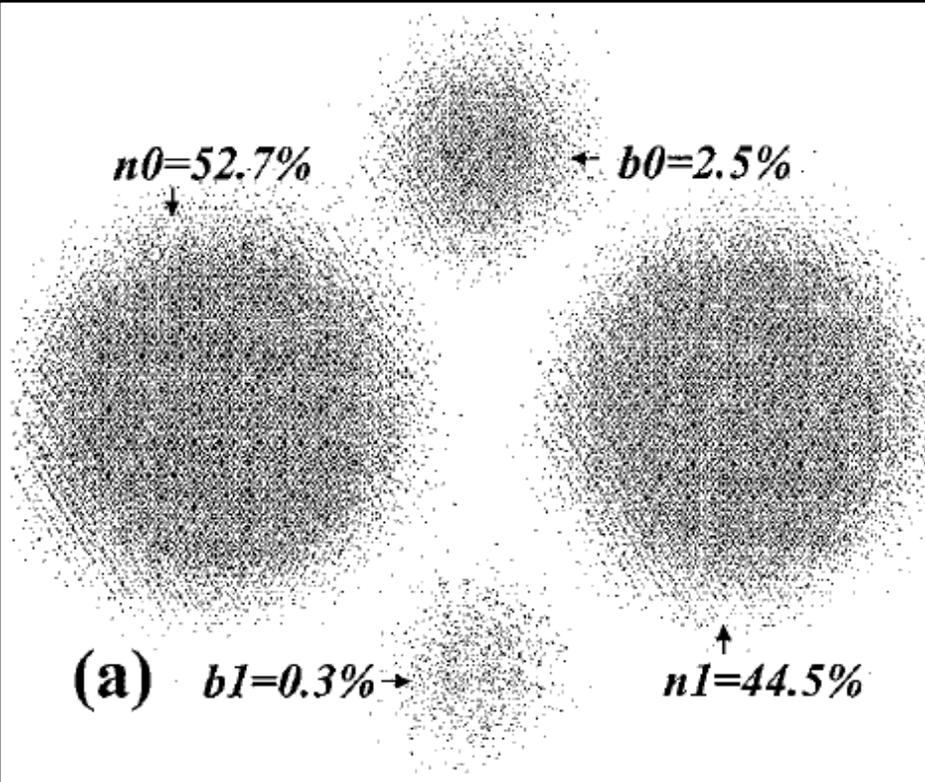




10^7 атомов



Вид в перпендикулярном пространстве



3d атомные поверхности в \perp пространстве

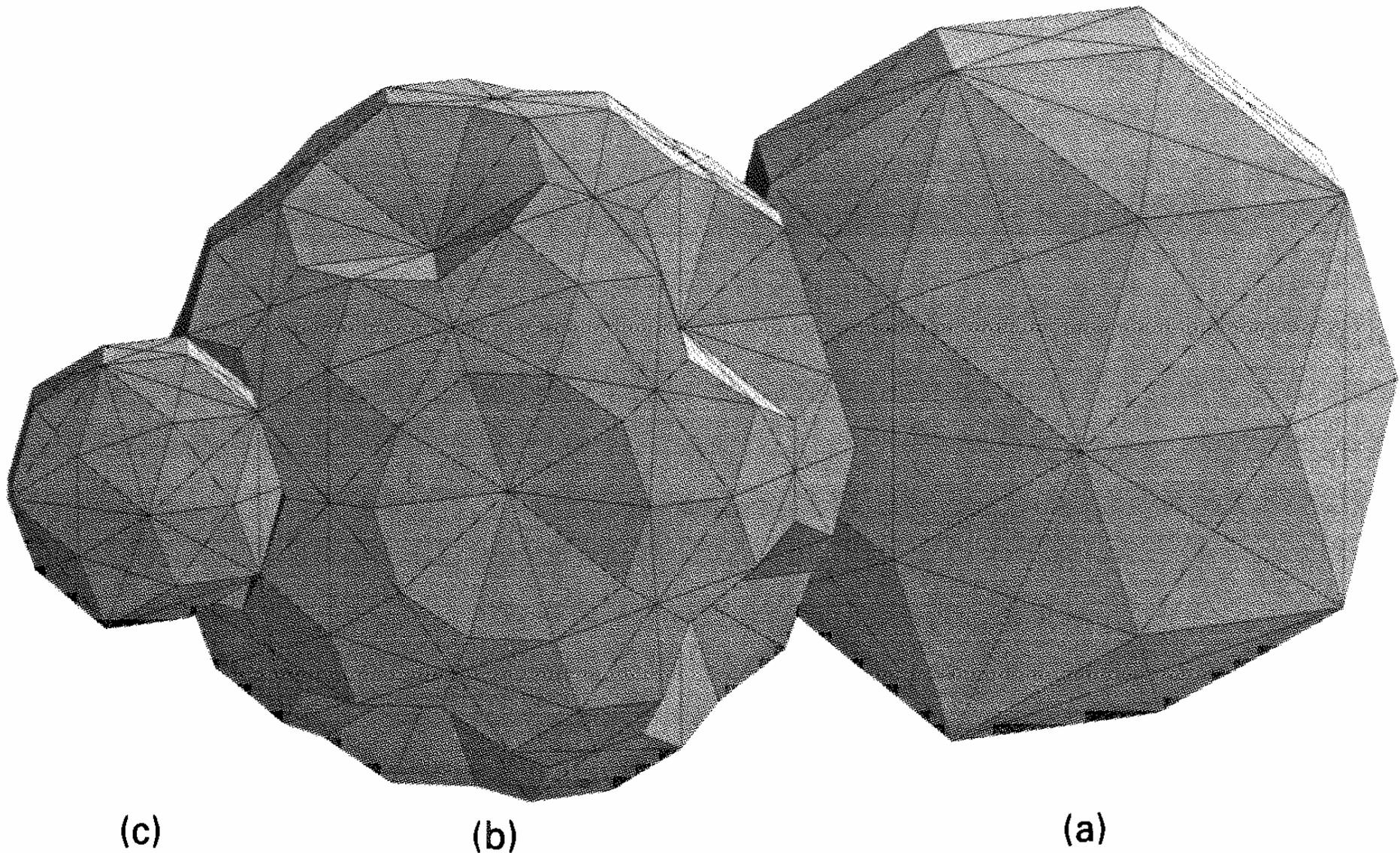


FIG. 4.24 Suggested atomic surfaces for the icosahedral AlFeCu system at sites (a) n_1 , (b) m_2 , and (c) bc_1 ^[31-33] (courtesy of M. Quiquandon).

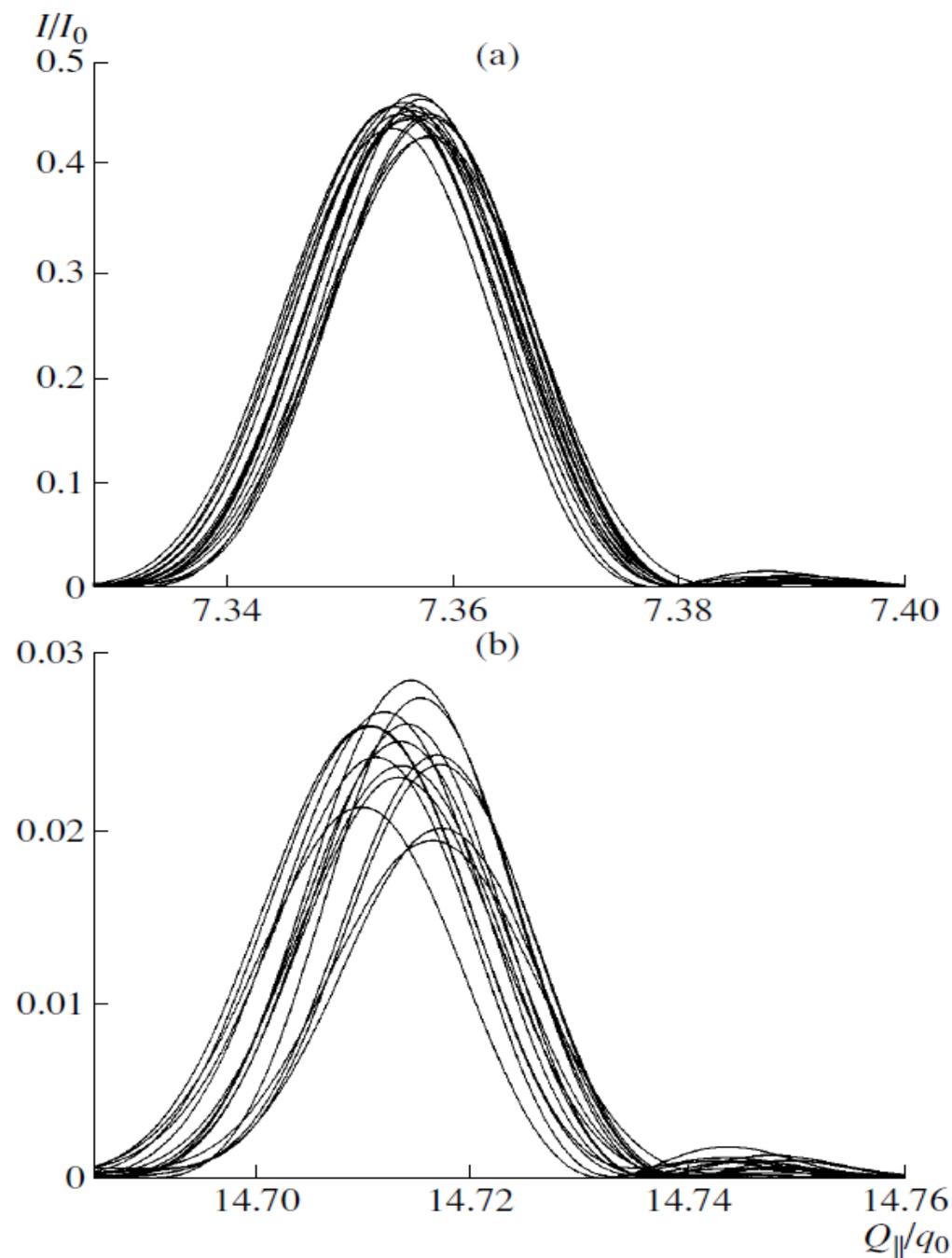


Fig. 3. Diffraction peaks along the twofold symmetry axes: (a) $(00001\bar{1})$ and (b) $(00002\bar{2})$. The curves were calculated along all the fifteen twofold axes.

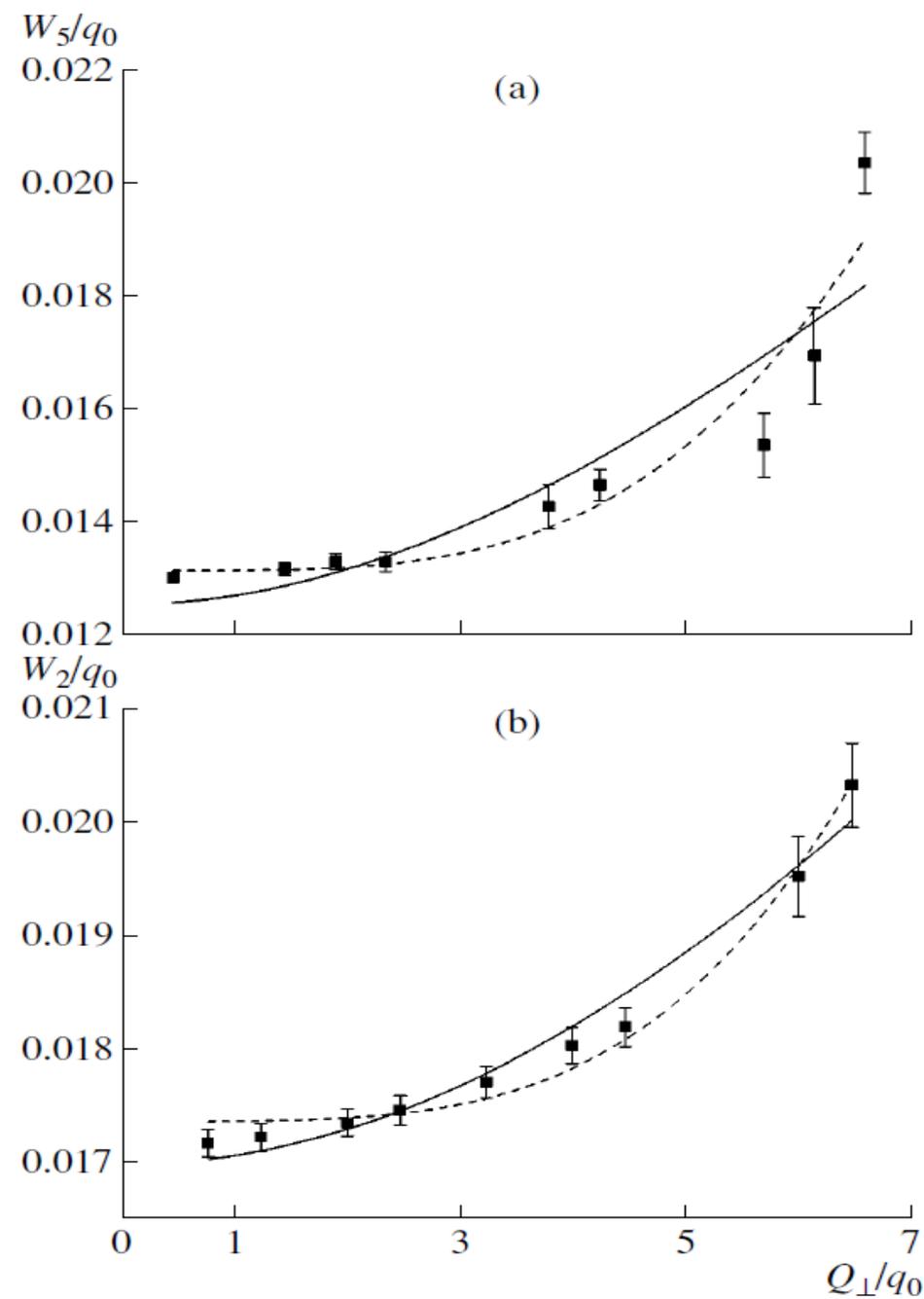
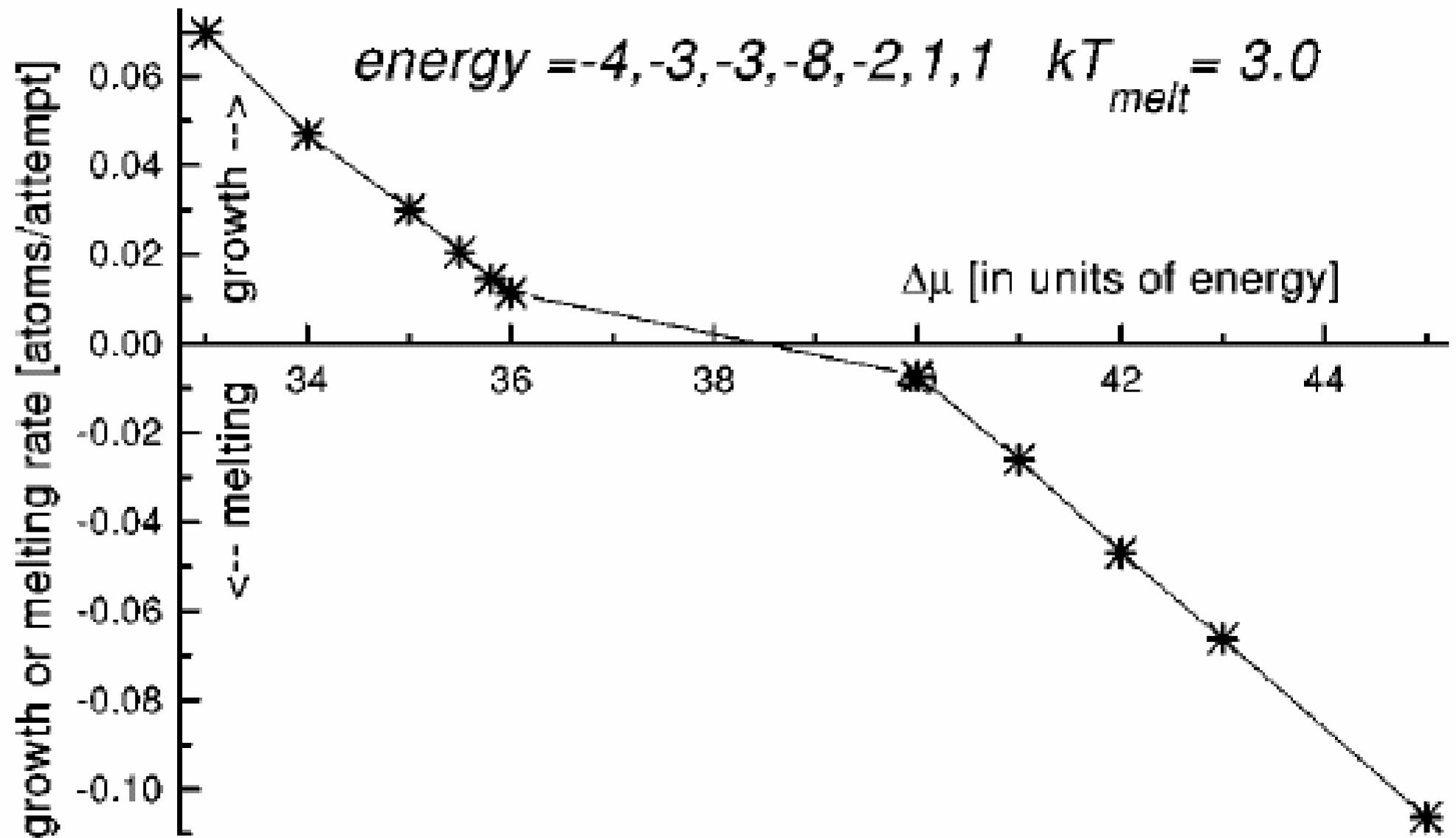


Fig. 4. Spectral width of reflections as a function of the magnitude of the perpendicular wave-vector component Q_{\perp} for reflections located along the (a) fivefold and (b) twofold



Скорость роста(плавления) в зависимости от
 переохлаждения(перегрева)

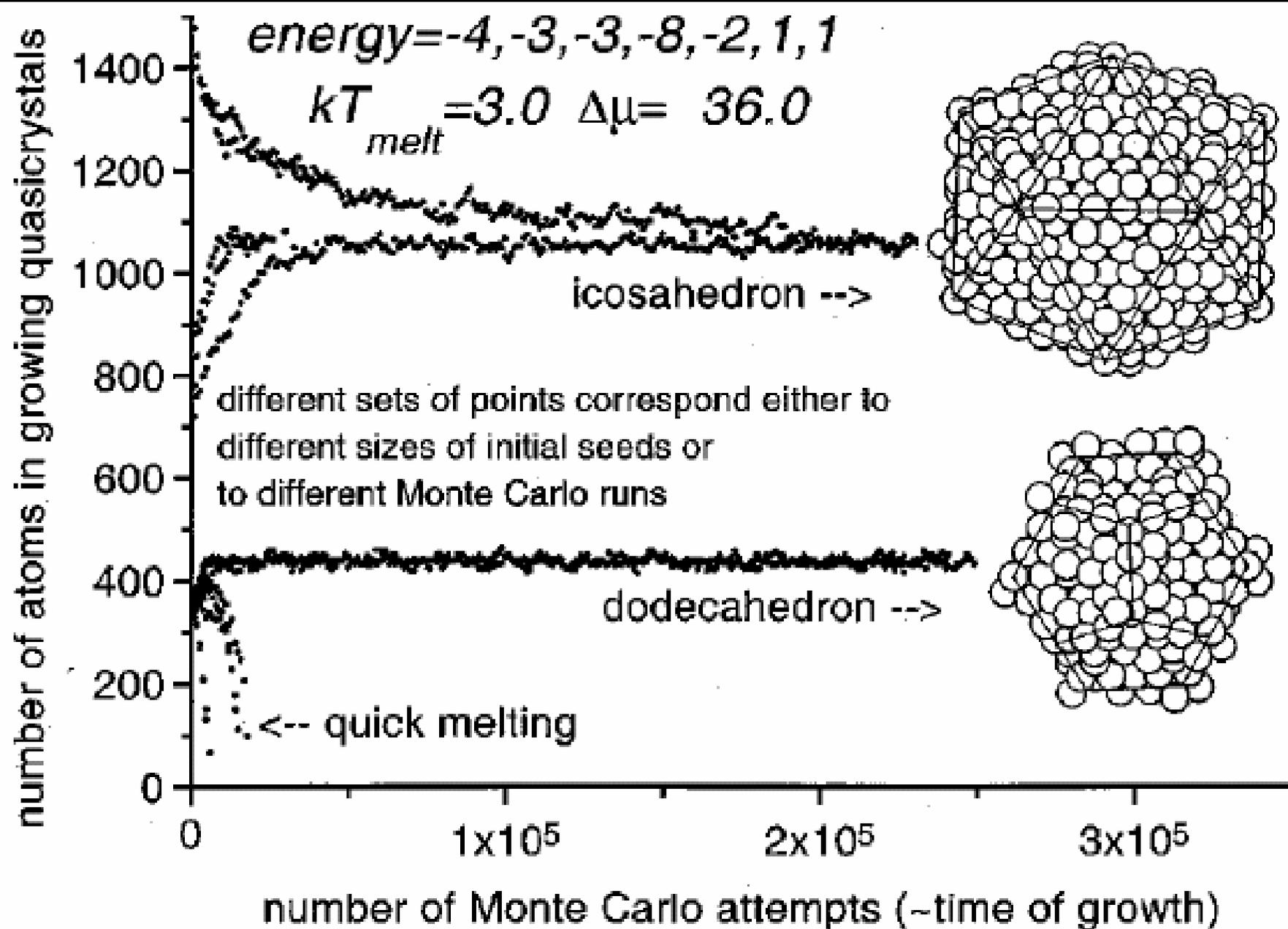


FIG. 7. Formation of stable clusters; different sets of points correspond either to different initial seeds or to different runs of the Monte Carlo process.

Благодарности

- Организаторам ФКС-2010
- Программе Президиума РАН «Физика сильно сжатого вещества и проблемы внутреннего строения Земли и планет»
- CNRS and IMPMC (Paris)
- соавторам: М.Клеман, Ф.Маури, С.Астафьев

Спасибо!

Conclusion

- displacements of atoms from their ideal positions grow with perpendicular radius
- the 2/1 approximants contain more body-centered (icosahedral) positions than “perfect” quasicrystals
- because of short distances and displacements, real-space methods for construction of higher approximants and quasicrystals should be developed

Аппроксиманты Фибоначчи

1/0: A.A.A.A.A.A.A.A подстановка: $A \rightarrow AB, B \rightarrow A$

1/1: AB.AB.AB.AB.AB.AB.AB.AB.AB

2/1: **ABA.ABA.ABA.ABA.ABA.ABA.ABA.ABA**

3/2: **ABAAB.ABAAB.ABAAB.ABAAB.ABAAB**

5/3: ABAABABA.ABAABABA.ABAABABA

τ : ABAABABA**ABAABABAABAABAABAABAABAABAABA**

Числа Фибоначчи: $F_{n+2} = F_{n+1} + F_n, F_0 = 0, F_1 = 1;$

0,1,2,3,5,8,13,21,34,55,89,... $\tau = (1 + 5^{1/2})/2 = 1.618034$

Аппроксиманты Фибоначчи

1/0: A.A.A.A.A.A.A.A подстановка: $A \rightarrow BA, B \rightarrow A$

1/1: BA.BA.BA.BA.BA.BA.BA.BA

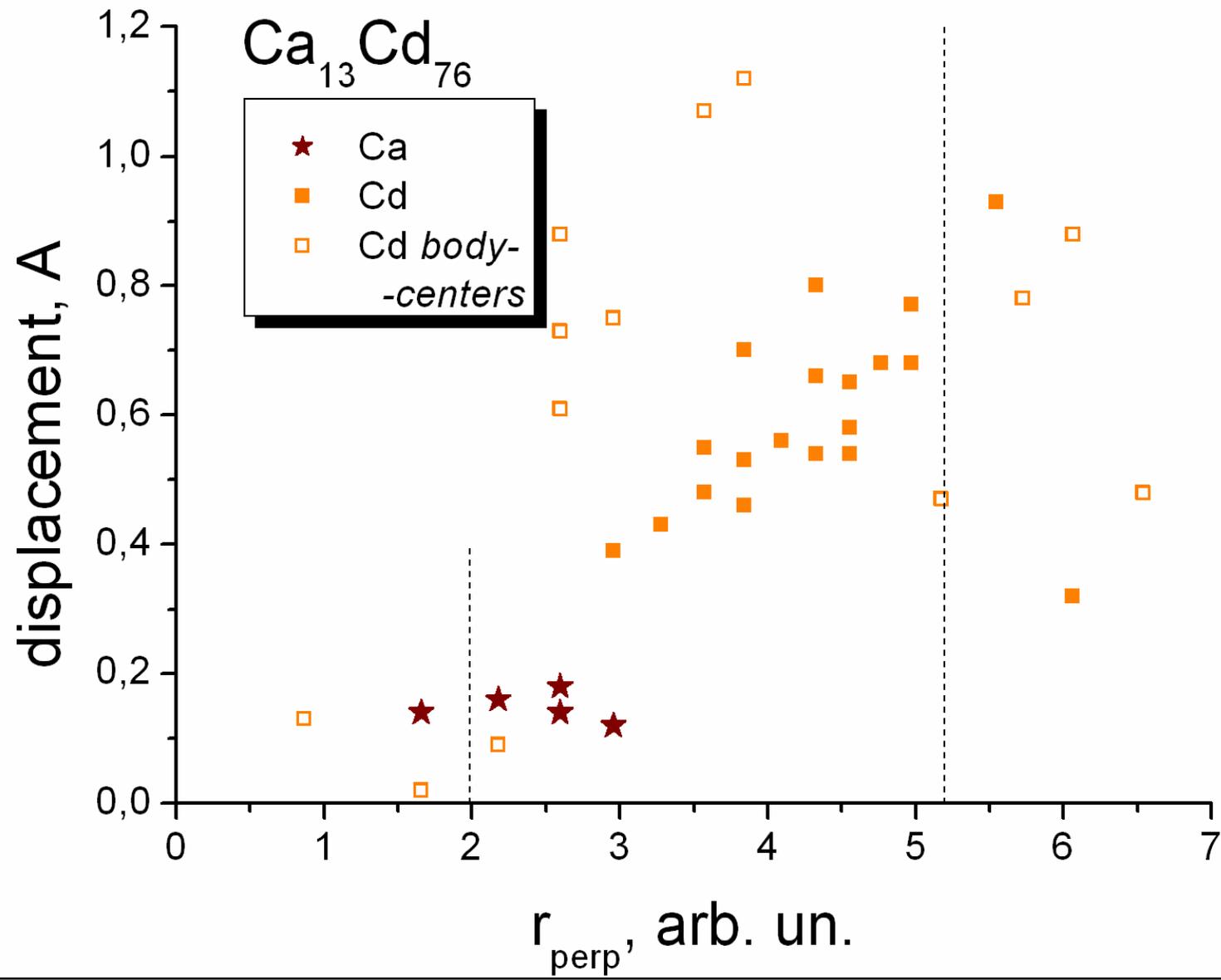
2/1: ABA.ABA.ABA.ABA.ABA.ABA

3/2: BAABA.BAABA.BAABA.BAABA

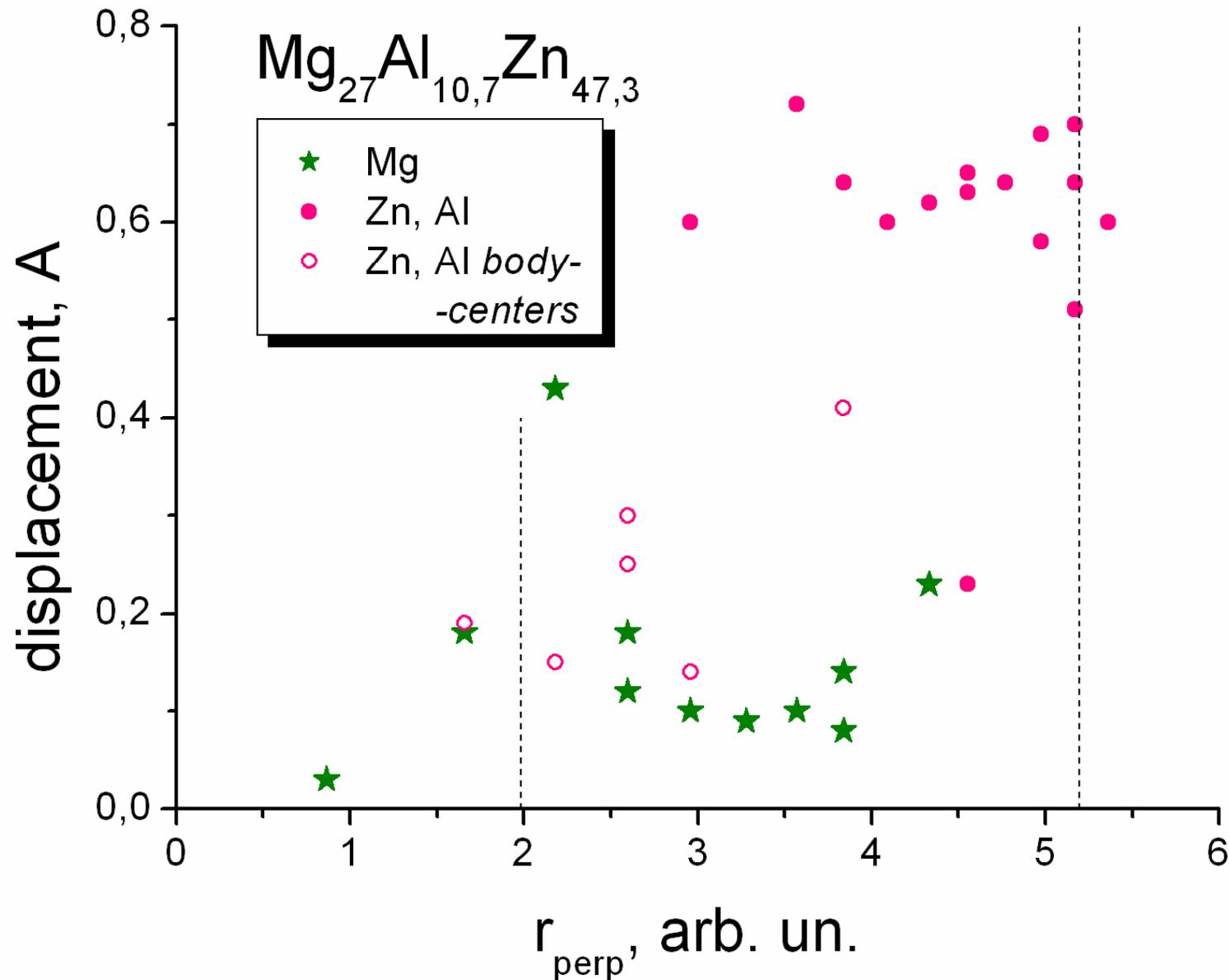
5/3: ABAABAABA.ABAABAABA

8/5: BAABAABAABA.BAABAABAABA

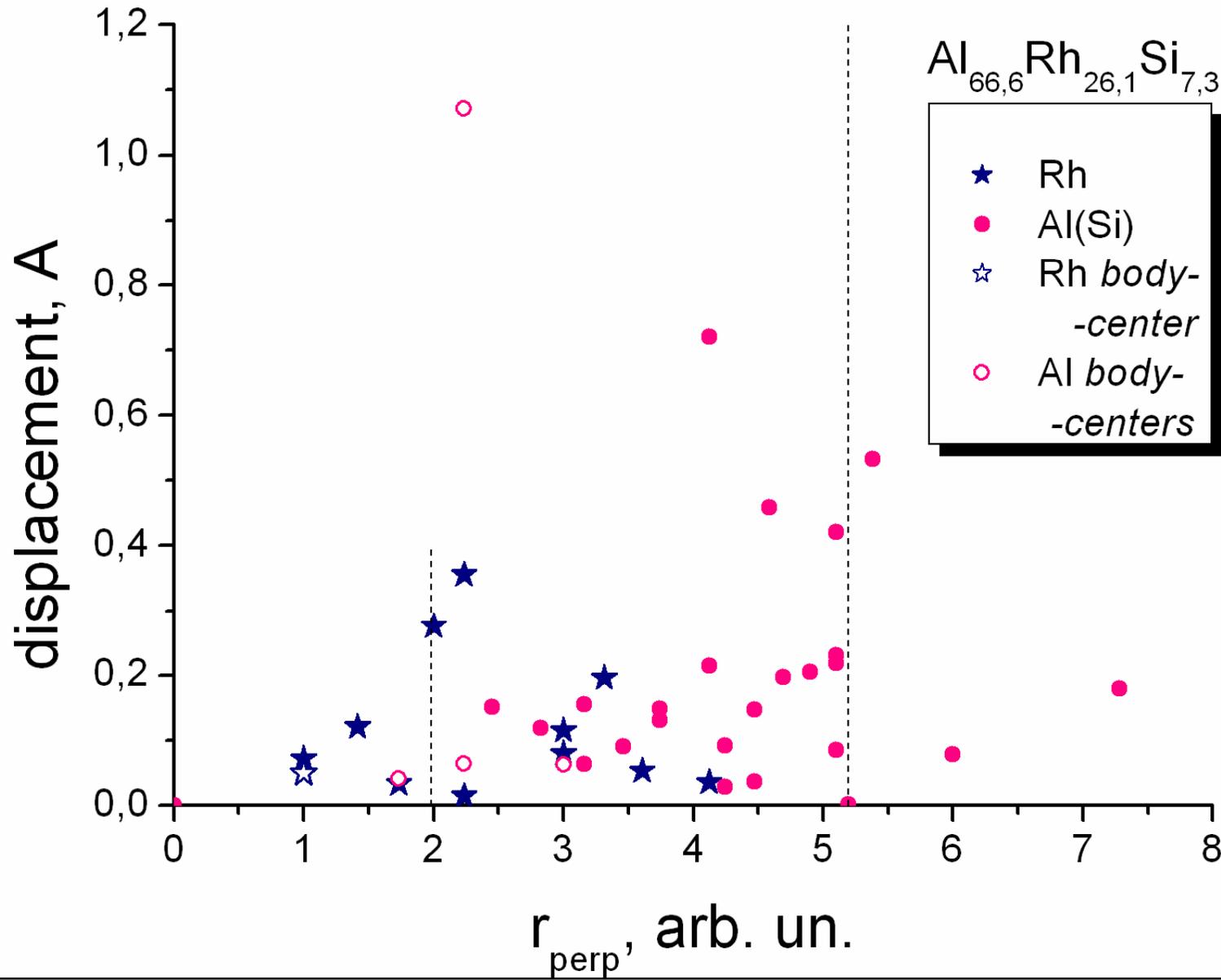
Displacements of atoms in real space *versus* their perpendicular positions: Ca-Cd



Displacements of atoms in real space *versus* their perpendicular positions: Mg-Al-Zn



Displacements of atoms in real space *versus* their perpendicular positions: Al-Rh-Si



Average characteristic of deviations from icosahedral symmetry in approximants

$$S = \left[\frac{\int f(\mathbf{r}\mathbf{e}'_2)^4 \rho(\mathbf{r}) d\mathbf{r} - \int f(\mathbf{r}\mathbf{e}_2)^4 \rho(\mathbf{r}) d\mathbf{r}}{\int f(\mathbf{r}\mathbf{e}_2)^4 \rho(\mathbf{r}) d\mathbf{r}} \right]^2,$$

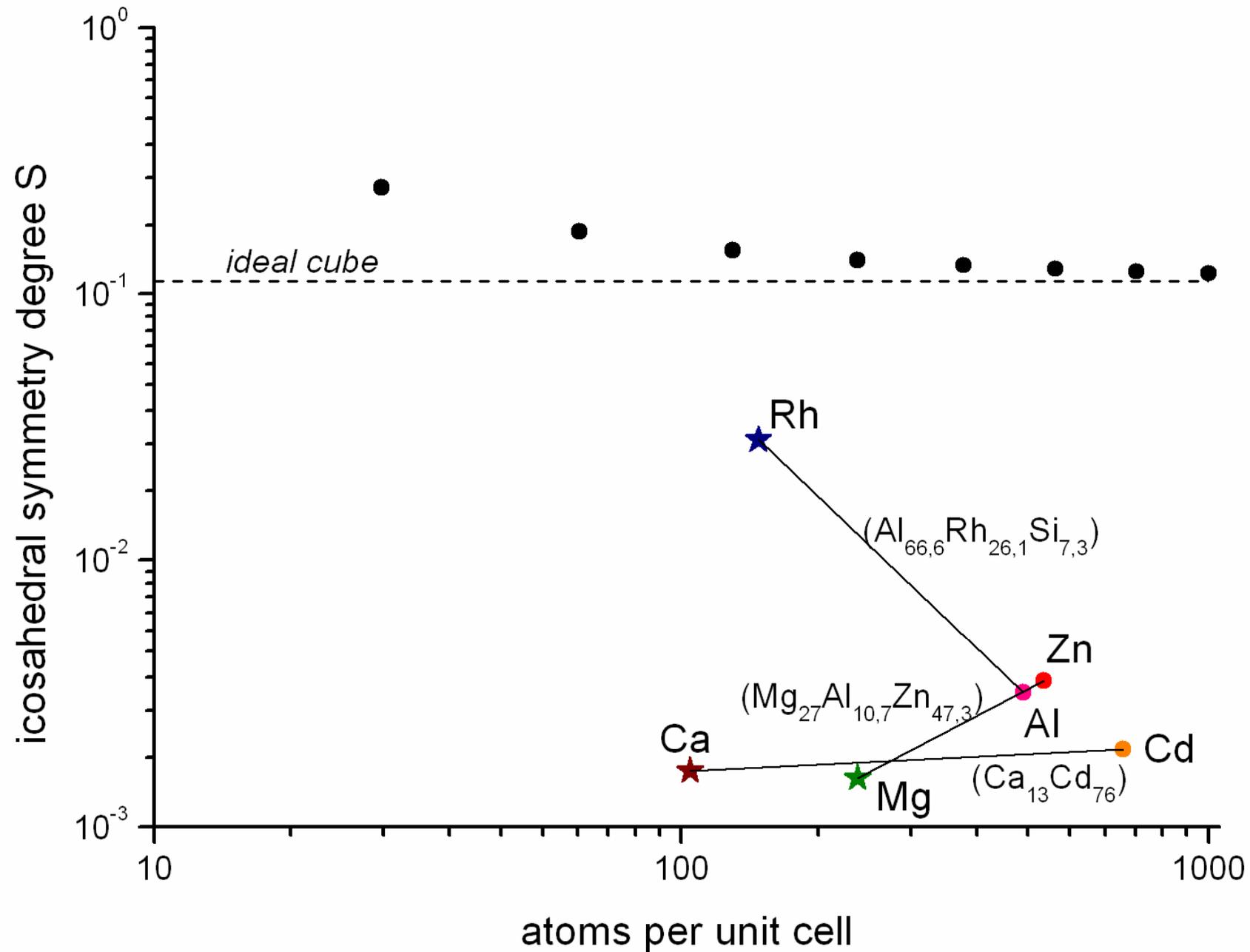
where $\rho(\mathbf{r})$ is the atomic density in the perpendicular space and

$$\mathbf{e}_2 = (1, 0, 0), \quad \mathbf{e}'_2 = \frac{1}{2}(\tau, \tau^{-1}, 1)$$

In cubic approximants

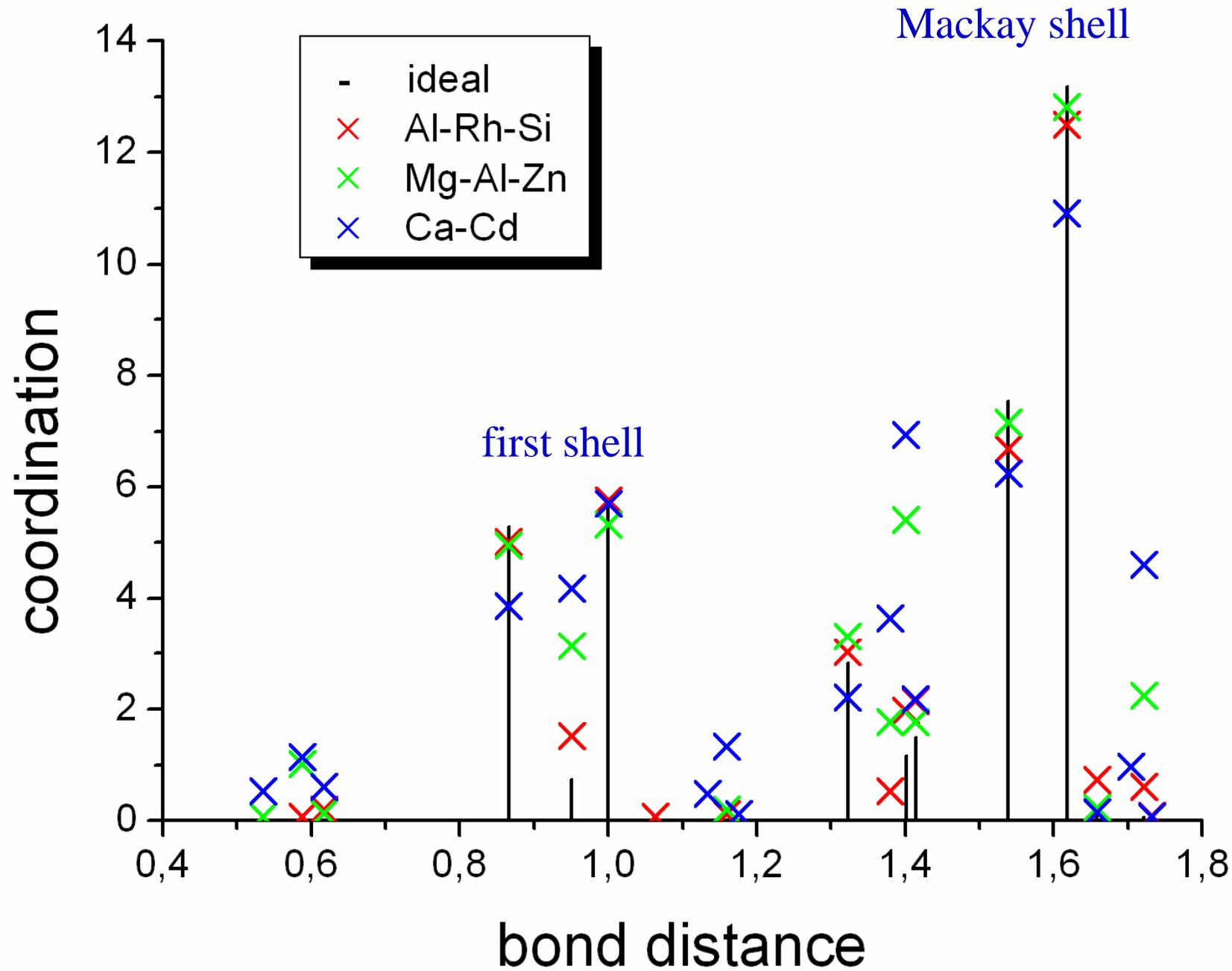
$$S = \left[\frac{3 \sum x^2 y^2}{2 \sum x^4} - \frac{1}{2} \right]^2$$

Characterization of icosahedral symmetry in approximants



Average coordination numbers of atoms in the 2/1 approximants

Approximants: Where are the atoms?



Real-space construction of higher approximants

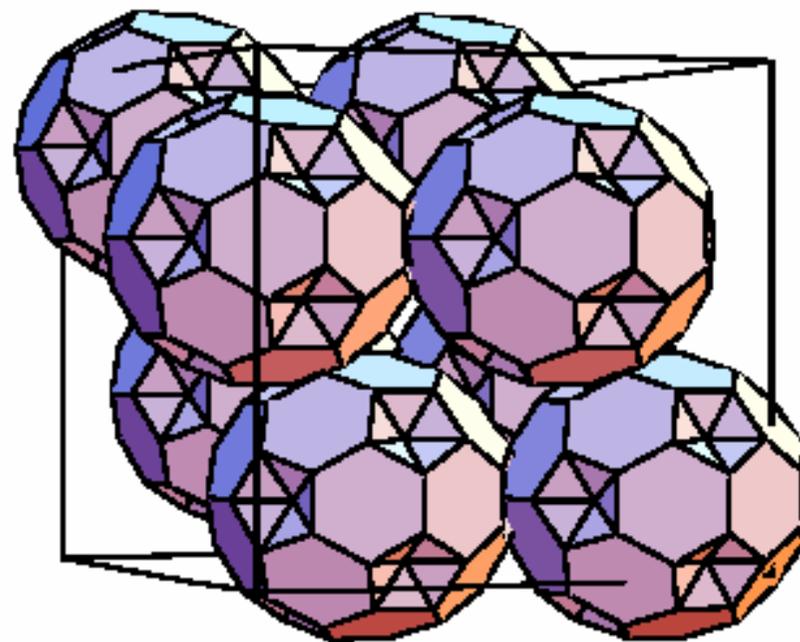
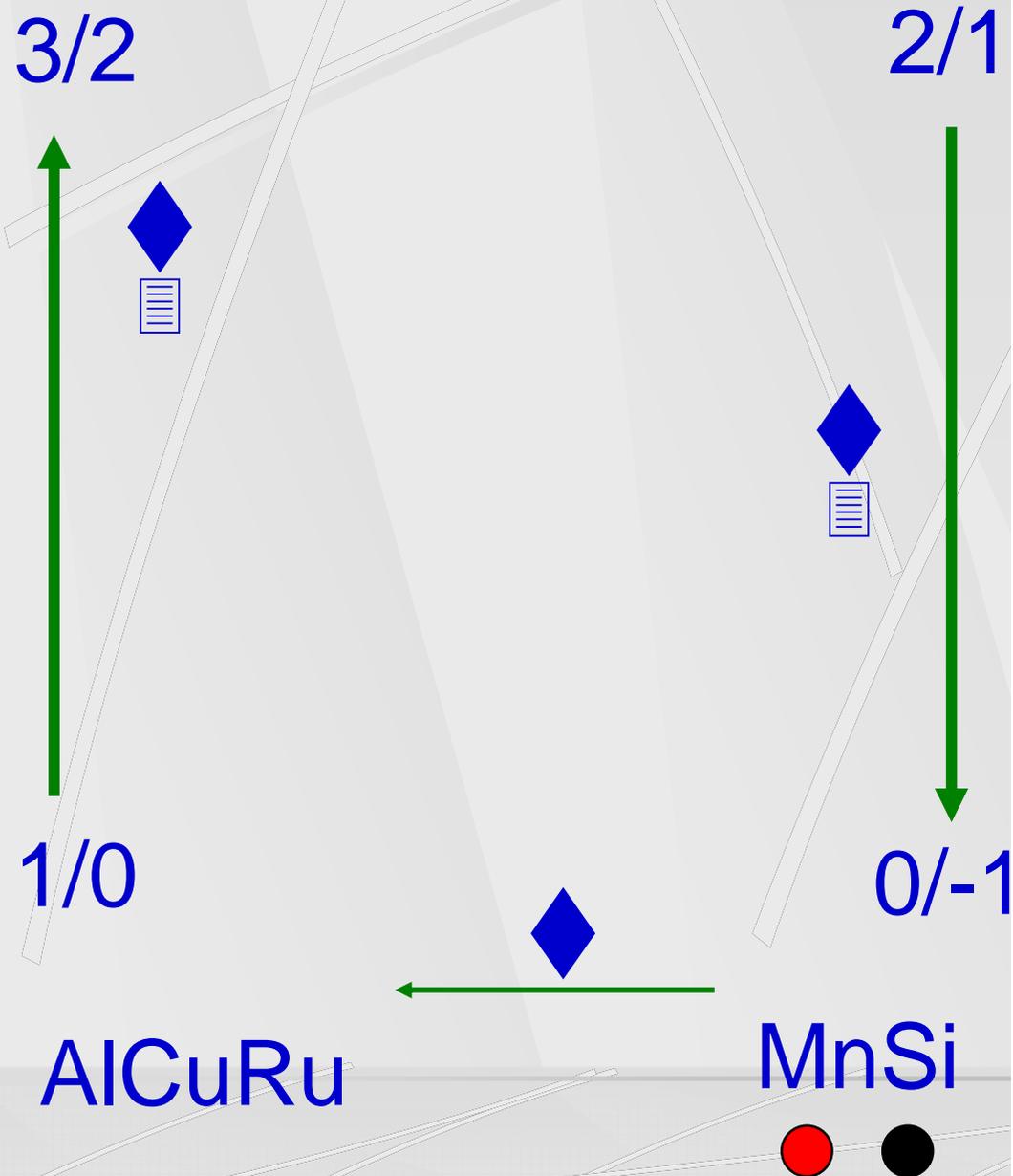


Fig. 1: Each unit cell of the 2/1-approximant contains eight Bergman clusters.

