Condensed Matter Physics

Crystal structure

Istvan Groma

ELTE

October 1, 2018

Periodic systems

Primitive lattice vectors

$$\underline{a}_1, \quad \underline{a}_2, \quad \underline{a}_3$$

Periodic systems

Primitive lattice vectors

$$\underline{a}_1, \quad \underline{a}_2, \quad \underline{a}_3$$

Bravais lattice

$$\underline{R}_n = n_1\underline{a}_1 + n_2\underline{a}_2 + n_3\underline{a}_3$$

Periodic systems

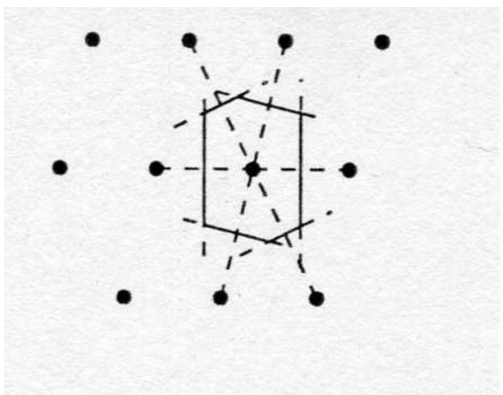
Primitive lattice vectors

$$\underline{a}_1, \quad \underline{a}_2, \quad \underline{a}_3$$

Bravais lattice

$$\underline{R}_n = n_1\underline{a}_1 + n_2\underline{a}_2 + n_3\underline{a}_3$$

Wigner-Seitz cell



Points and directions

Bravais lattice points

$$\underline{r} = x_1\underline{a}_1 + x_2\underline{a}_2 + x_3\underline{a}_3$$

$$\left(\frac{1}{2}, \frac{\bar{1}}{2}, 0\right)$$

Points and directions

Bravais lattice points

$$\underline{r} = x_1\underline{a}_1 + x_2\underline{a}_2 + x_3\underline{a}_3$$

$$\left(\frac{1}{2}, \frac{\bar{1}}{2}, 0\right)$$

Directions

$$u\underline{a}_1 + v\underline{a}_2 + w\underline{a}_3$$

$$[u, v, w]$$

Points and directions

Bravais lattice points

$$\underline{r} = x_1\underline{a}_1 + x_2\underline{a}_2 + x_3\underline{a}_3$$

$$\left(\frac{1}{2}, \frac{\bar{1}}{2}, 0\right)$$

Directions

$$u\underline{a}_1 + v\underline{a}_2 + w\underline{a}_3$$

$$[u, v, w]$$

Reciprocal lattice

$$\underline{a}_{1,2,3} \rightarrow \underline{b}_{1,2,3} \qquad \underline{a}_i\underline{b}_j = 2\pi\delta_{ij}$$

$$\underline{b}_1 = 2\pi\frac{\underline{a}_2 \times \underline{a}_3}{det} \qquad \underline{b}_2 = 2\pi\frac{\underline{a}_3 \times \underline{a}_1}{det} \qquad \underline{b}_3 = 2\pi\frac{\underline{a}_1 \times \underline{a}_2}{det}$$

Points and directions

$$\begin{pmatrix} a_{1x} & a_{2x} & a_{3x} \\ a_{1y} & a_{2y} & a_{3y} \\ a_{1z} & a_{2z} & a_{3z} \end{pmatrix} \begin{pmatrix} b_{1x} & b_{1y} & b_{1z} \\ b_{2x} & b_{2y} & b_{2z} \\ b_{3x} & b_{3y} & b_{3z} \end{pmatrix} = \begin{pmatrix} 2\pi & & \\ & 2\pi & \\ & & 2\pi \end{pmatrix}$$

$$v_r = \frac{(2\pi)^3}{v_c}$$

Brilluen zone = reciprocal Wigner Seitz cell

Points and directions

$$\begin{pmatrix} a_{1x} & a_{2x} & a_{3x} \\ a_{1y} & a_{2y} & a_{3y} \\ a_{1z} & a_{2z} & a_{3z} \end{pmatrix} \begin{pmatrix} b_{1x} & b_{1y} & b_{1z} \\ b_{2x} & b_{2y} & b_{2z} \\ b_{3x} & b_{3y} & b_{3z} \end{pmatrix} = \begin{pmatrix} 2\pi & & \\ & 2\pi & \\ & & 2\pi \end{pmatrix}$$

$$v_r = \frac{(2\pi)^3}{v_c}$$

Brilluen zone = reciprocal Wigner Seitz cell

Miller index

$$\underline{G}_{hkl} = h\underline{b}_1 + k\underline{b}_2 + l\underline{b}_3 \qquad (h, k, l)$$

Points and directions

$$\begin{pmatrix} a_{1x} & a_{2x} & a_{3x} \\ a_{1y} & a_{2y} & a_{3y} \\ a_{1z} & a_{2z} & a_{3z} \end{pmatrix} \begin{pmatrix} b_{1x} & b_{1y} & b_{1z} \\ b_{2x} & b_{2y} & b_{2z} \\ b_{3x} & b_{3y} & b_{3z} \end{pmatrix} = \begin{pmatrix} 2\pi & & \\ & 2\pi & \\ & & 2\pi \end{pmatrix}$$

$$v_r = \frac{(2\pi)^3}{v_c}$$

Brilluen zone = reciprocal Wigner Seitz cell

Miller index

$$\underline{G}_{hkl} = h\underline{b}_1 + k\underline{b}_2 + l\underline{b}_3 \qquad (h,k,l)$$

Equation for a plane

$$\underline{r}\,\underline{G}_{hkl} = const.$$

Crosses

$$\underline{R}_n = n_1\underline{a}_1 + n_2\underline{a}_2 + n_3\underline{a}_3$$

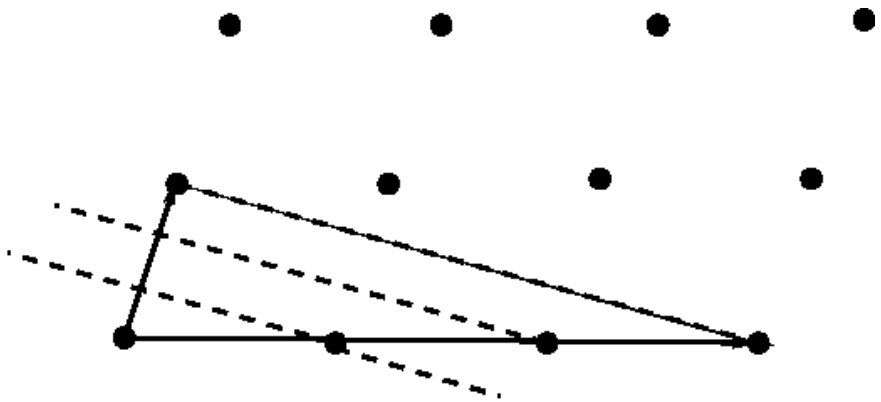
$$const. = 2\pi m$$

Points and directions

$$h * x_1 + k * x_2 + l * x_3 = m$$

Intercepts

$$\frac{m}{h}, \quad \frac{m}{k}, \quad \frac{m}{l},$$



Distance of the planes

$$d = \underline{a}_1 \frac{(m+1) - m}{h} \frac{\underline{G}_{hkl}}{|\underline{G}_{hkl}|} = \frac{2\pi}{|\underline{G}_{hkl}|}$$

Rotation of the crystal

Köbös kristály

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Rotation of the crystal

Köbös kristály

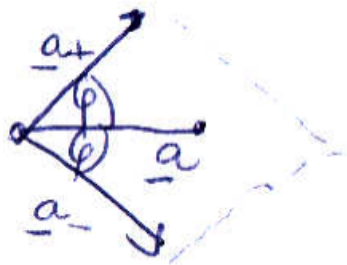
$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Rotation of the crystal

Köbös kristály

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Rotation



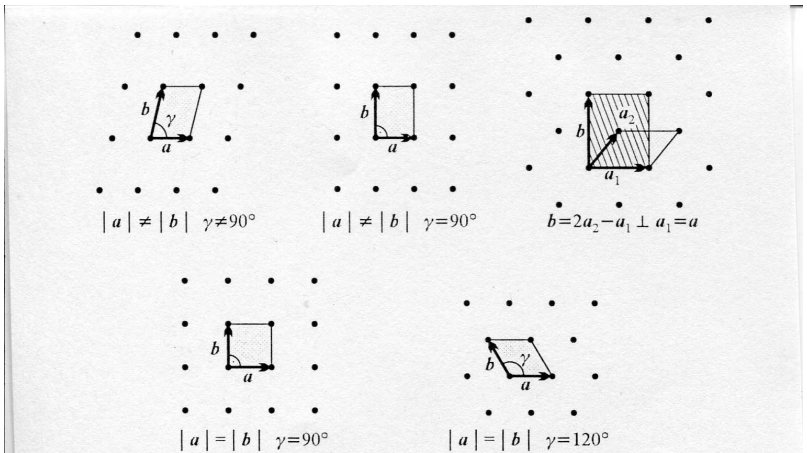
$$\underline{a}_+ + \underline{a}_- = m\underline{a}$$

$$\underline{a}_+ + \underline{a}_- = (2\cos(\varphi), 0, 0)a$$

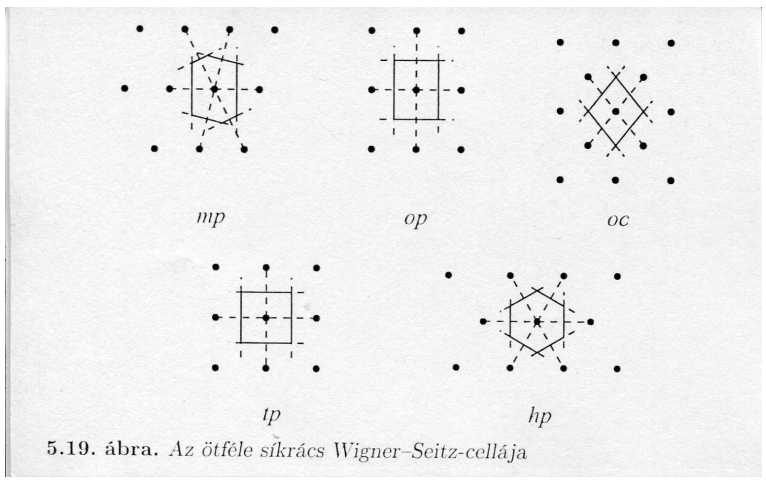
$$\cos(\varphi) = 0, \quad \pm\frac{1}{2}, \quad \pm 1$$

$$\varphi = 0, \quad \pm\frac{2\pi}{2}, \quad \pm\frac{2\pi}{3}, \quad \pm\frac{2\pi}{4}, \quad \pm\frac{2\pi}{6}$$

2D crystals

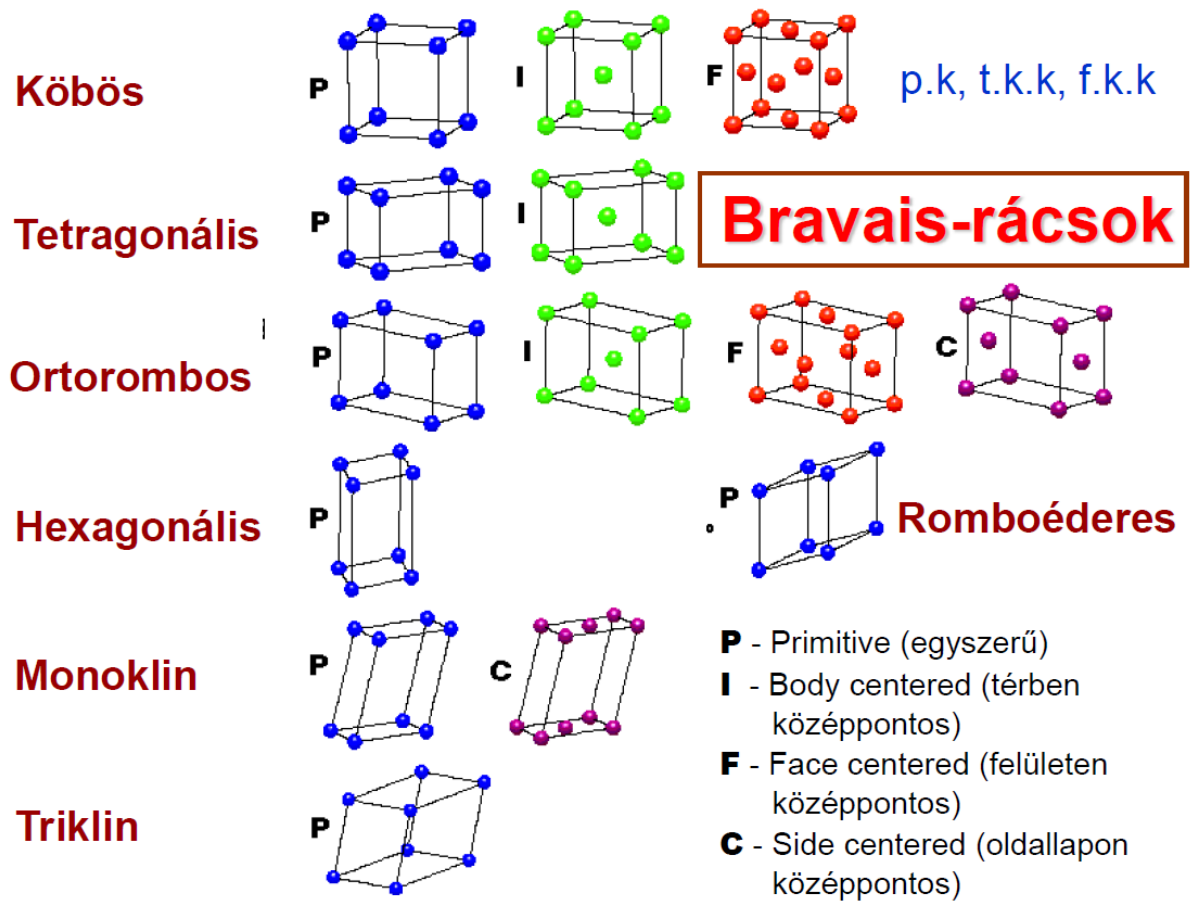


5.18. ábra. *A kétdimenziós kristályszerkezetben lehetséges Bravais-rács típusok és elemi cellájuk. A centrált derékszögű rácsnál a Bravais-cellát is megadjuk*

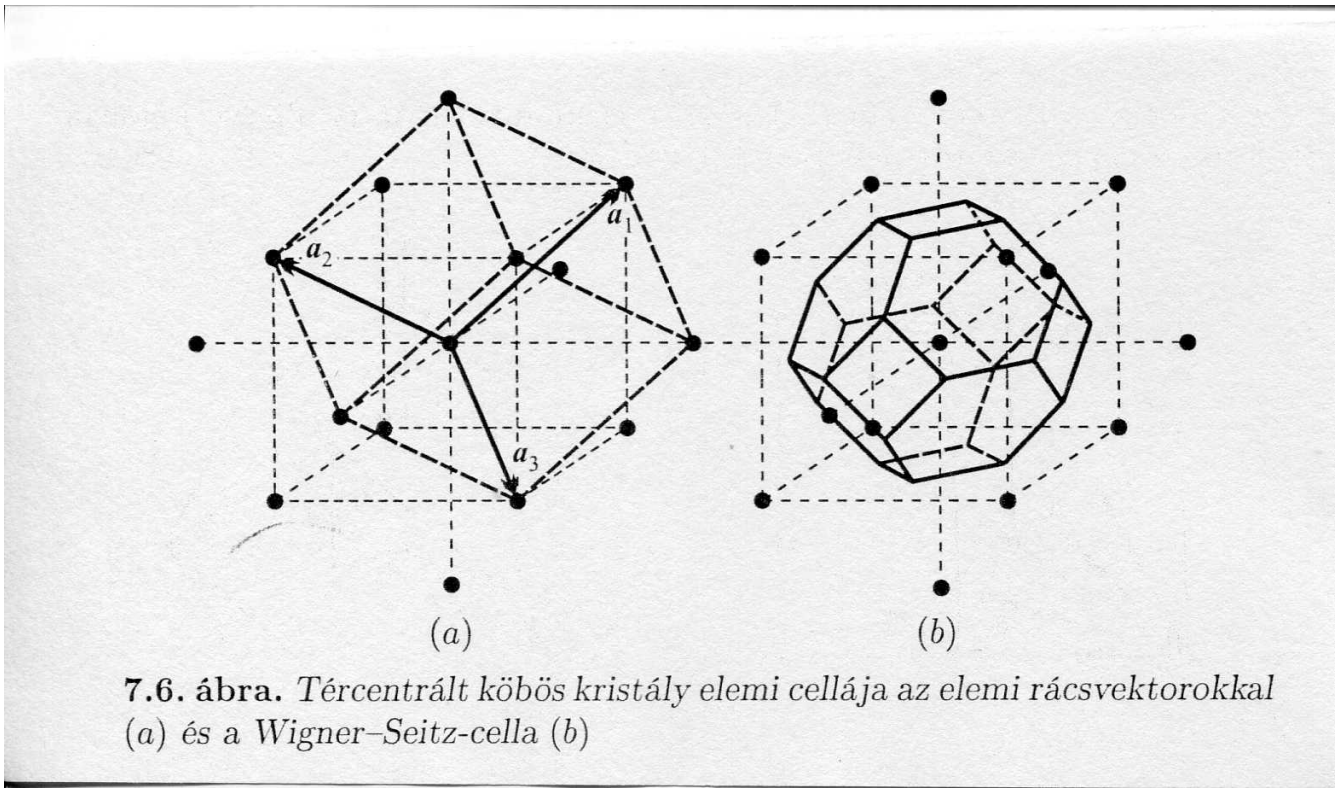


5.19. ábra. *Az ötféle síkrács Wigner–Seitz-cellája*

3D crystals


Köbös
P
I
F
p.k, t.k.k, f.k.k
Tetragonális
P
I
Bravais-rácsok
Ortorombos
P
I
F
C
Hexagonális
P
P
Romboéderes
Monoklin
P
C
Triklin
P
P - Primitive (egyszerű)
I - Body centered (térben középpontos)
F - Face centered (felületen középpontos)
C - Side centered (oldallapon középpontos)

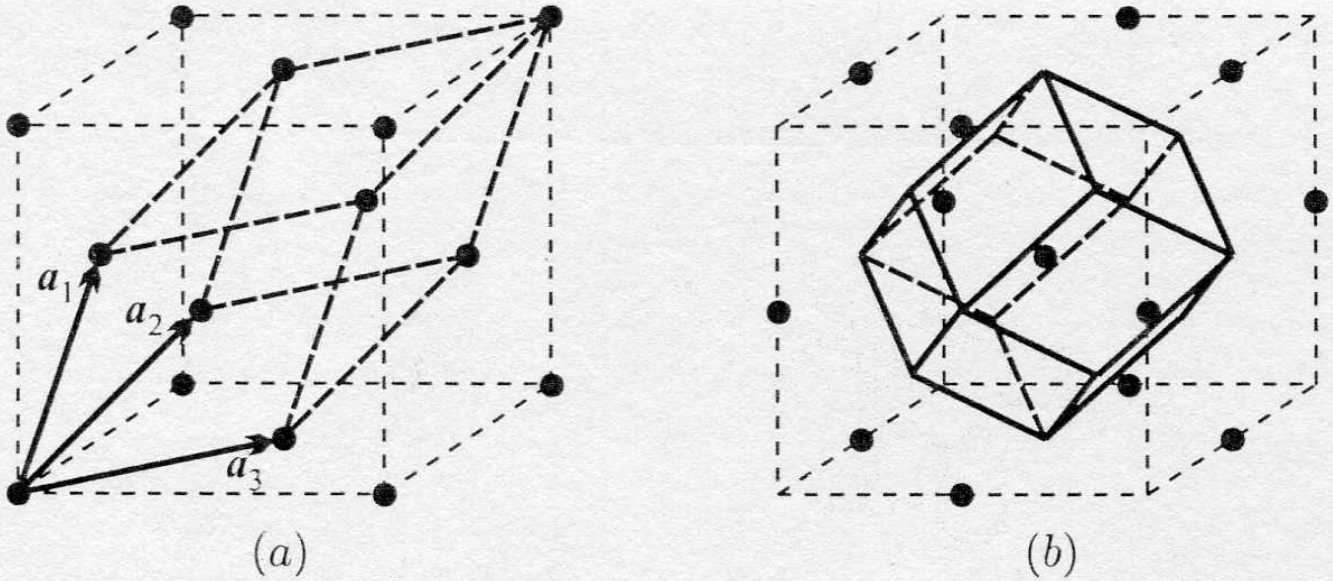
BCC



7.6. ábra. *Tércentrált köbös kristály elemi cellája az elemi rácsvektorokkal (a) és a Wigner–Seitz-cella (b)*

Cr, Fe, Mo, Nb

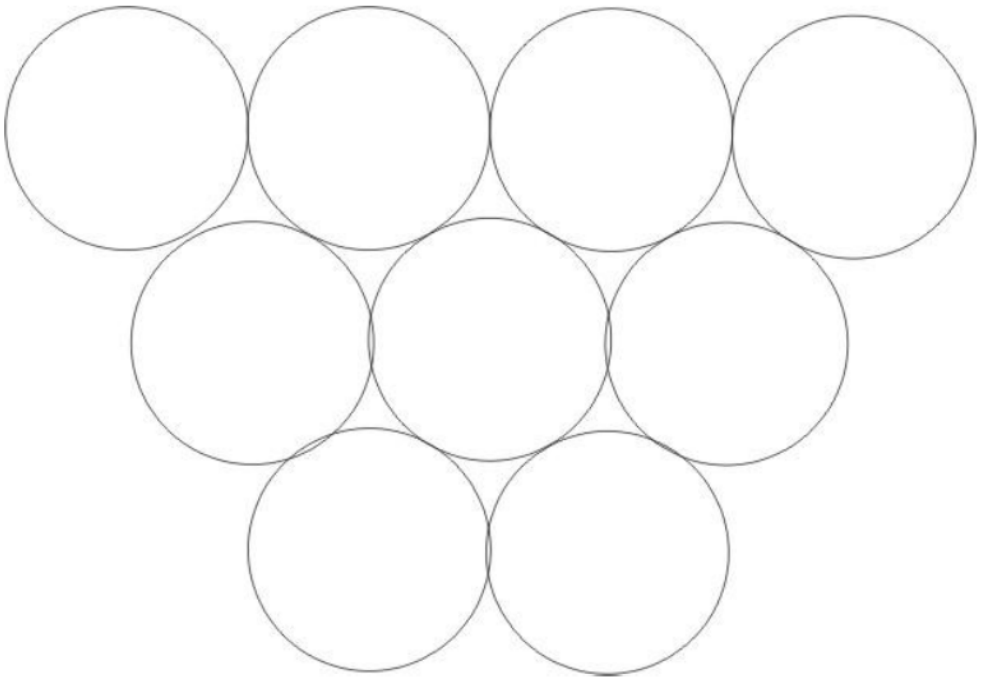
FCC



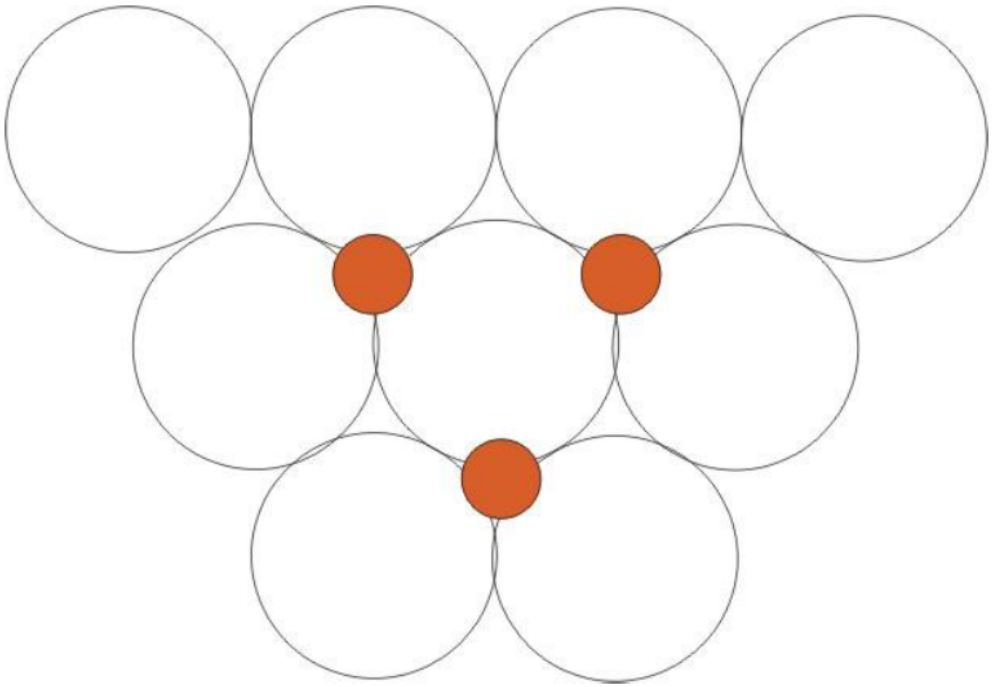
7.9. ábra. *Lapcentrált köbös kristály Bravais-cellája az elemi rácsvektorokkal (a) és Wigner–Seitz-cellája (b)*

Cu, Ag, An, Ni

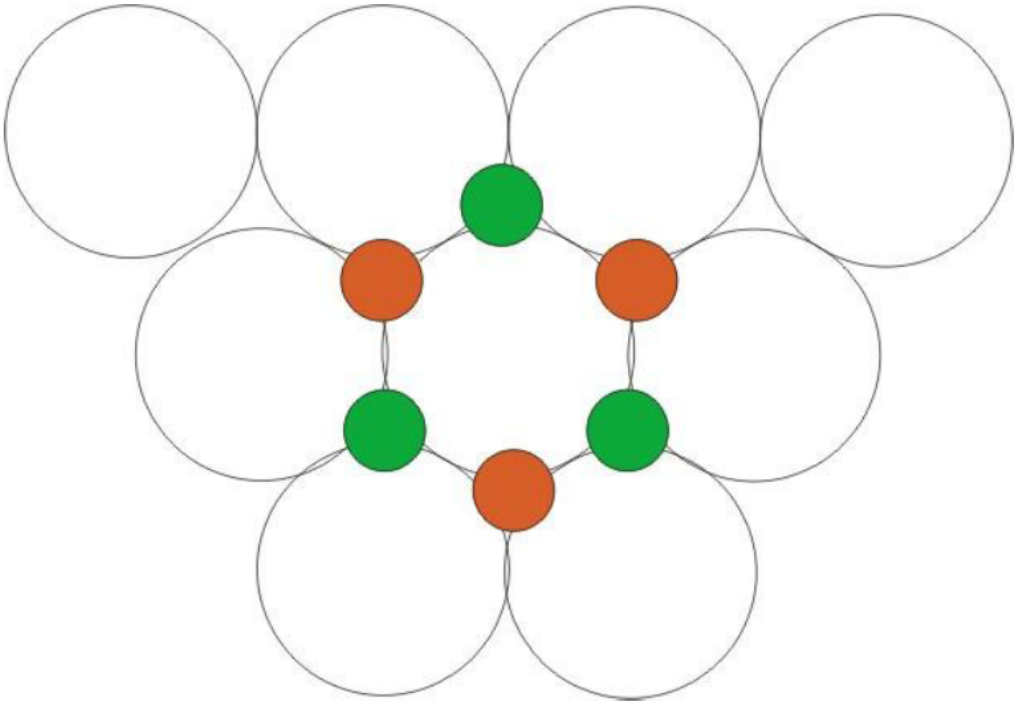
Closed packed crystals



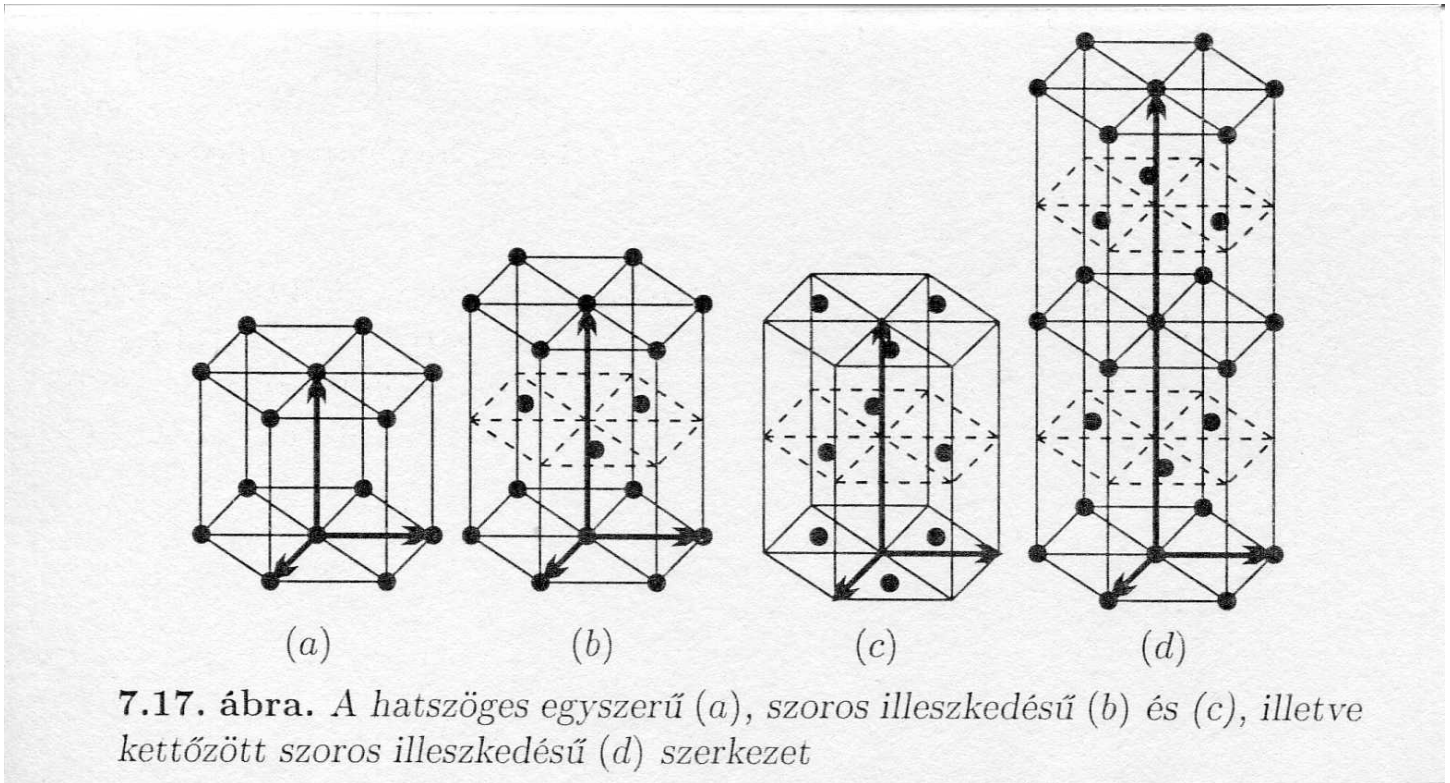
Closed packed crystals



Closed packed crystals



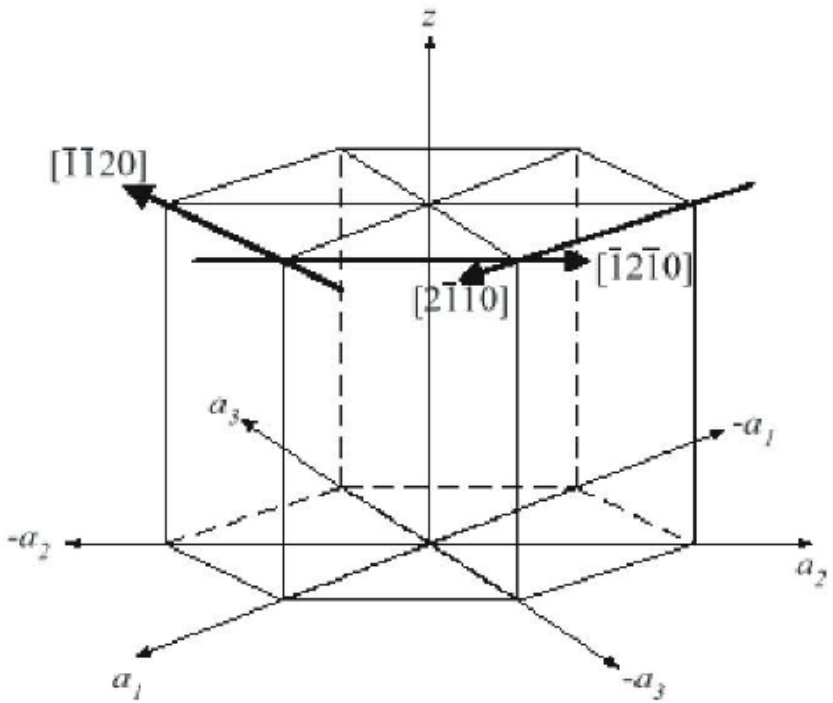
HCP



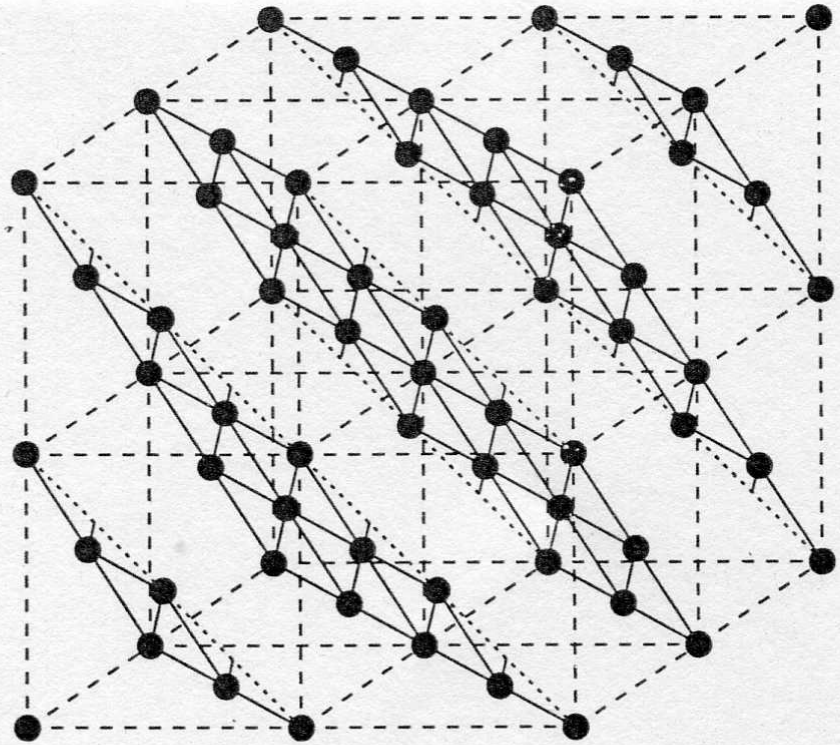
7.17. ábra. *A hatszöges egyszerű (a), szoros illeszkedésű (b) és (c), illetve kettőzött szoros illeszkedésű (d) szerkezet*

Co, Ti, Zn, Ni, Mg

HCP

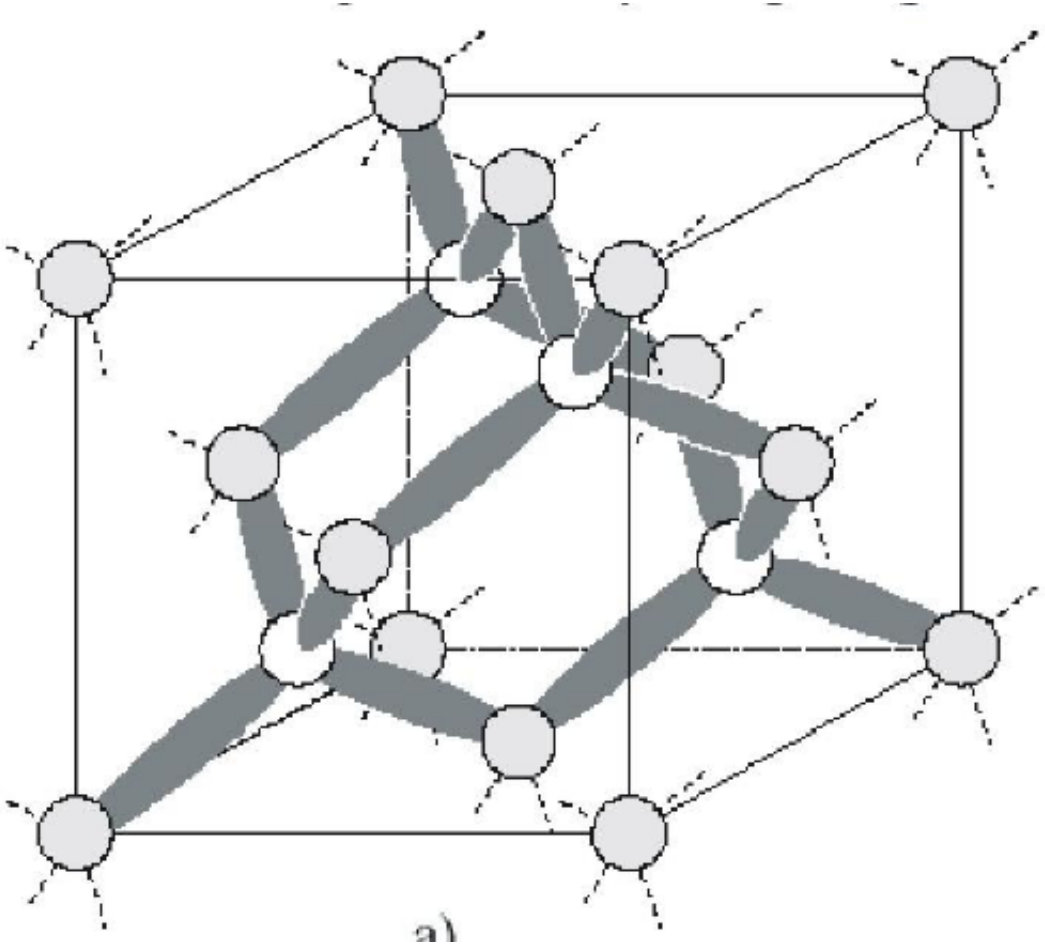


FCC closed packing

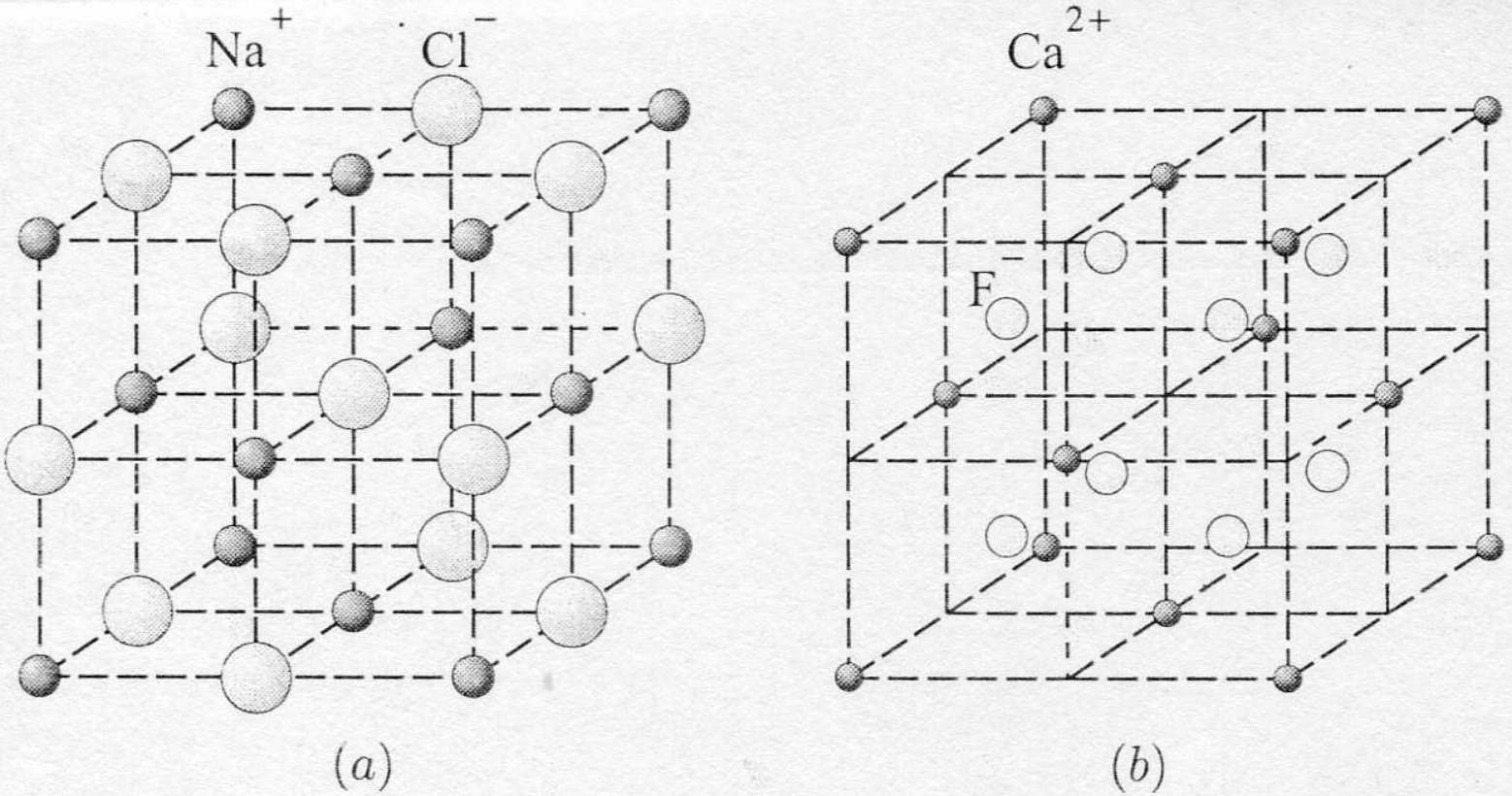


7.11. ábra. *Az atomok szoros illeszkedésű elhelyezkedése lapcentrált köbös kristályban a térátlóra merőleges síkokban*

Diamond crystal



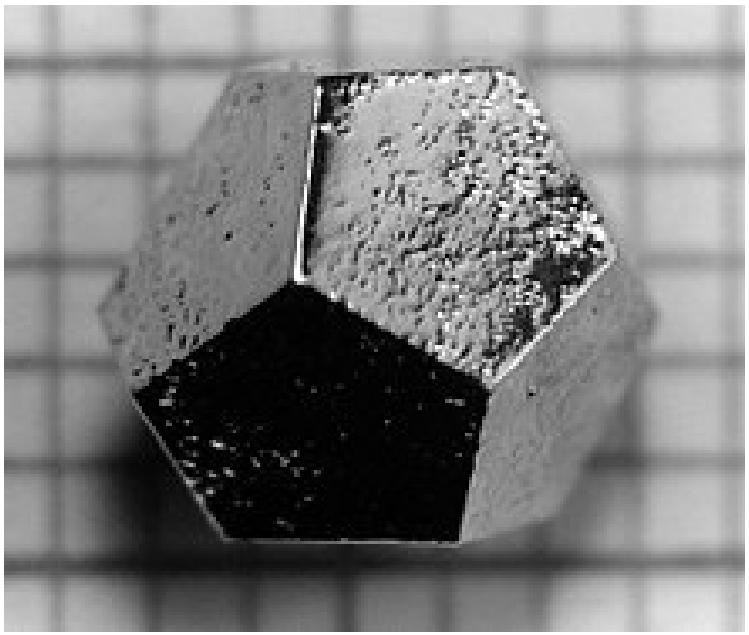
Systems with more atom



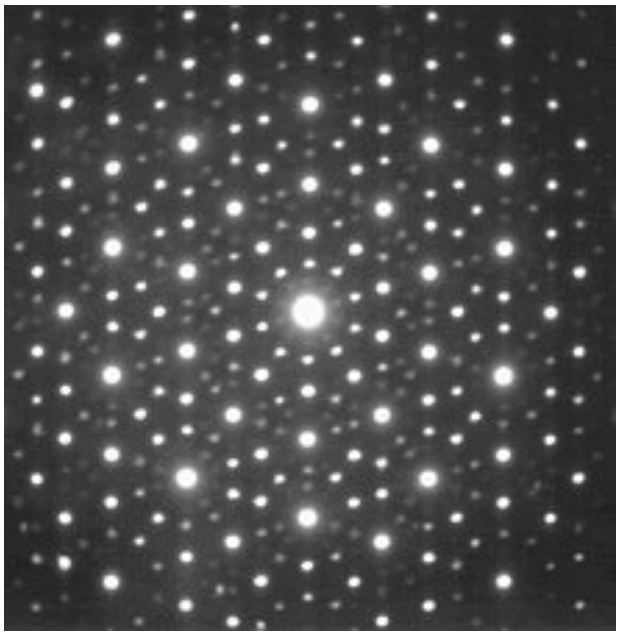
7.13. ábra. *Kősó típusú (B1) (a) és fluorit típusú (C1) (b) kristályszerkezet*

Quasicrystal

Daniel Dan Shechtman (1982), Nobel price 2011

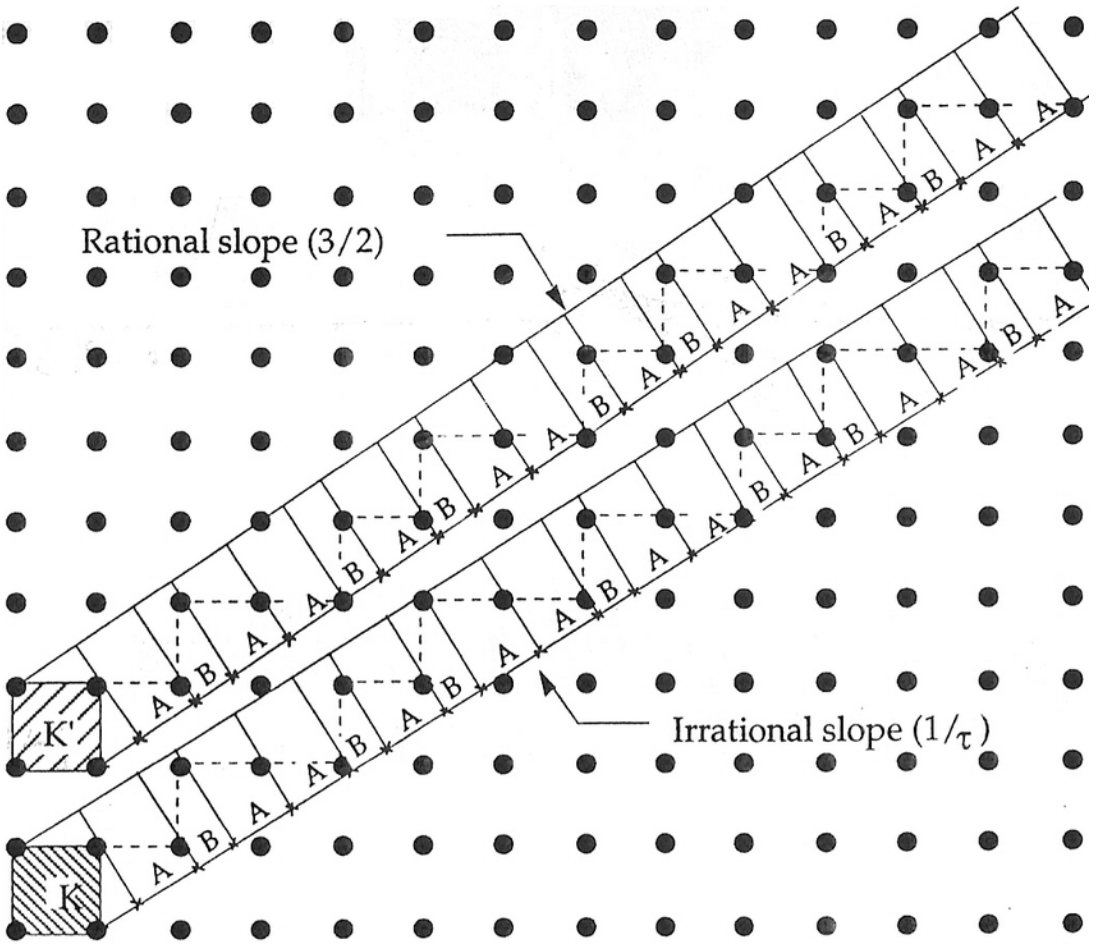


Quasicrystal



Diffraction image

Construction

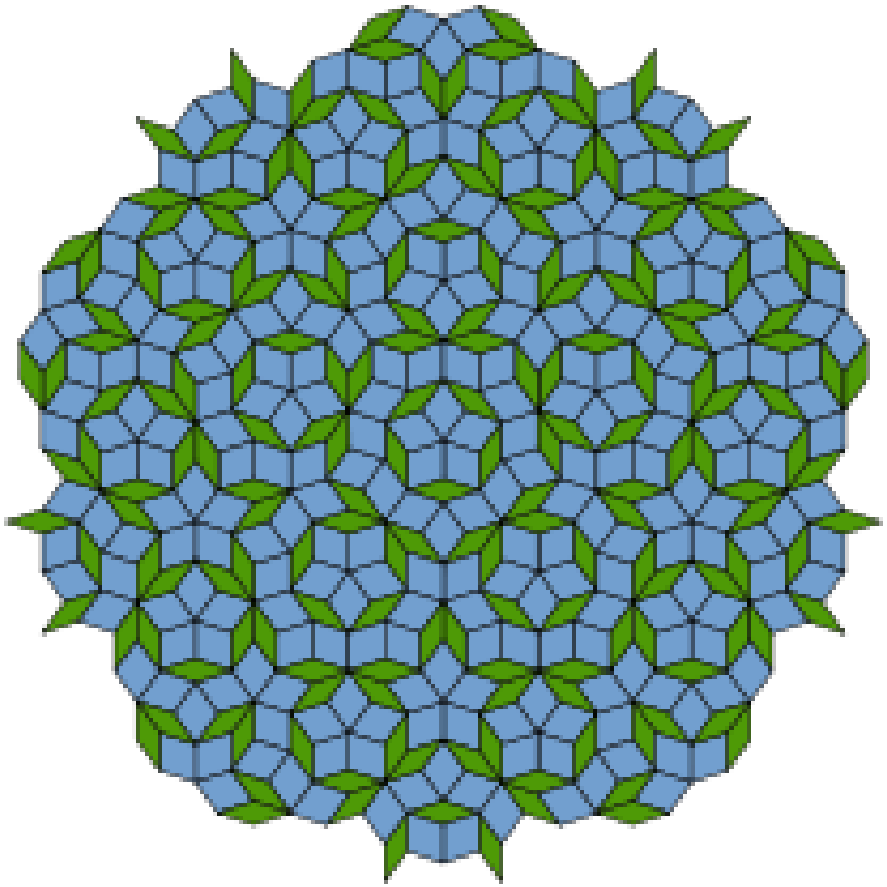


Construction

Table 4. The Fibonacci chain.

Fibonacci number	Fibonacci sequence	#L	#S
1	S	0	1
1	L	1	0
2	LS	1	1
3	LSL	2	1
5	LSLLS	3	2
8	LSLLSLSL	5	3
13	LSLLSLSLLSLLS	8	5
21	LSLLSLSLLSLLSLSLLSLSL	13	8
...	.....	...	...

2D Quasicrystal



Penrose tiling
Fat rhombus 72, 72, 108, 108 angles
Slim rhombus 36, 36, 144, 144 angles