



Anyagtudomány

Rácsszerkezetek

Groma István

ELTE

March 29, 2021



<http://metal.elte.hu/groma/Anyagtudomany/>

Charles Kittel: Introduction to Solid State Physics

Sólyom Jenő: A modern szilárdtest-fizika alapjai I

R.W. Chan: Physical Metallurgy



Elemi rácsvektorok

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



Elemi rácsvektorok

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



Bravais Rács

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

Elemi rácsvektorok

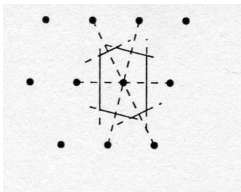
$$\underline{a}_1, \underline{a}_2, \underline{a}_3$$



Bravais Rács

Wigner-Seitz cella

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



Bravais rácspont

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

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

Bravais rácspont

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

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

Irányok

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

$$[u, v, w]$$

Bravais rácspont

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

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

Írányok

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

$$[u, v, w]$$

Reciprok rács

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

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

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

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

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

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

Brilluen zóna = reciprokrács Wigner Seitz cellája

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

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Miller index

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

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

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Miller index

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

Sík egyenlete

$$\underline{rG}_{hkl} = \text{const.}$$

Átmegy

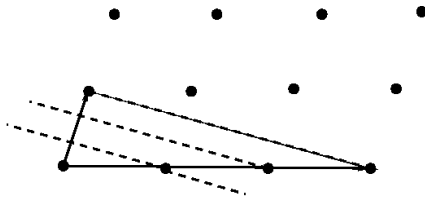
$$\underline{R}_n = n_1\underline{a}_1 + n_2\underline{a}_2 + n_3\underline{a}_3$$

$$\text{const.} = 2\pi m$$

Tengelymetszetek

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

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



Síkok távolsága

$$d = a_1 \frac{(m+1) - m}{h} \frac{G_{hkl}}{|G_{hkl}|} = \frac{2\pi}{|G_{hkl}|}$$

Köbös kristály

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

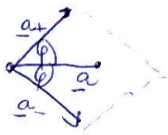
Köbös kristály

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

Köbös kristály

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

Kristály elforgatása

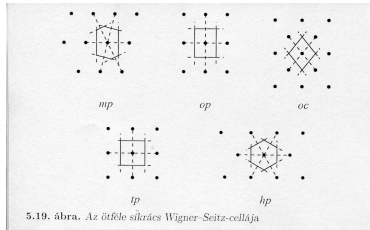
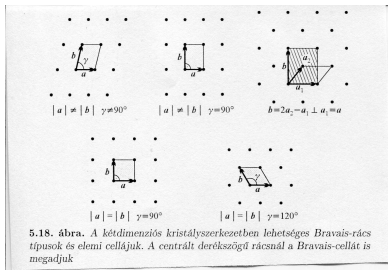


$$\underline{a}_+ + \underline{a}_- = m\underline{a}$$

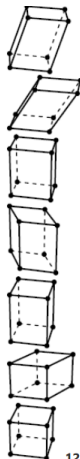
$$\underline{a}_+ + \underline{a}_- = (2 \cos(\varphi), 0, 0)a$$

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

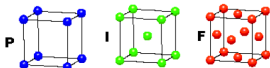
$$\varphi = 0, \pm \frac{2\pi}{2}, \pm \frac{2\pi}{3}, \pm \frac{2\pi}{4}, \pm \frac{2\pi}{6}$$



• Triklin	1 cella (P)	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
• Monoklin	2 cella (P, C)	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$
• Rombos	4 cella (P, C, I, F)	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
• Hatszögös	1 cella (P)	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$
• Négyzetes	2 cella (P, I)	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
• Romboédères	1 cella (R)	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$
• Köbös	3 cella (P, I, F)	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$

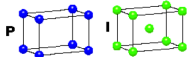


Köbös



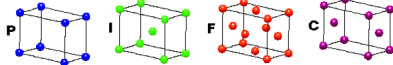
p.k, t.k.k, f.k.k

Tetragonális



Bravais-rácsok

Ortorombos

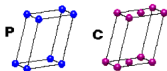


Hexagonális



Romboédes

Monoklin



Triklin

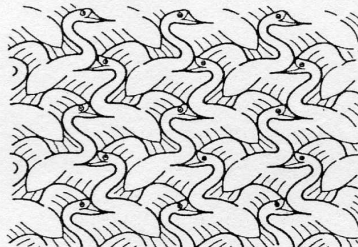
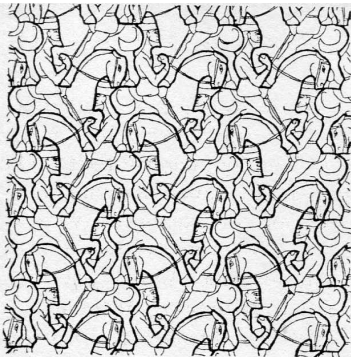


P - Primitive (egyszerű)

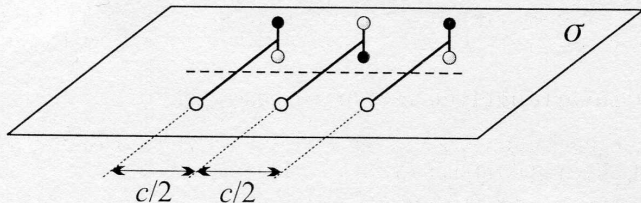
I - Body centered (térben középpontos)

F - Face centered (felületen középpontos)

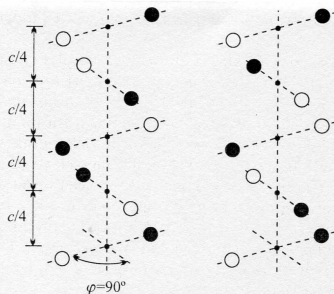
C - Side centered (oldallapon középpontos)



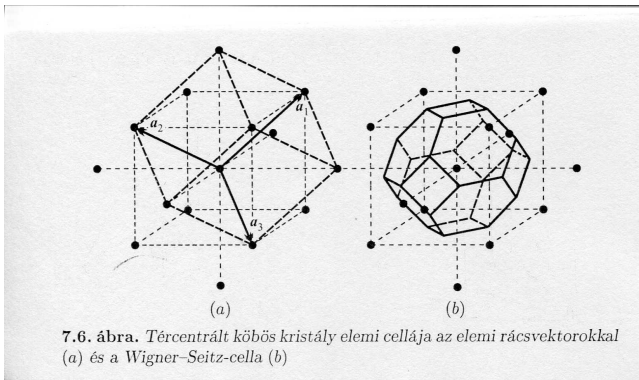
5.26. ábra. Csúszóvonalal rendelkező síkbeli alakzatok Escher rajzain



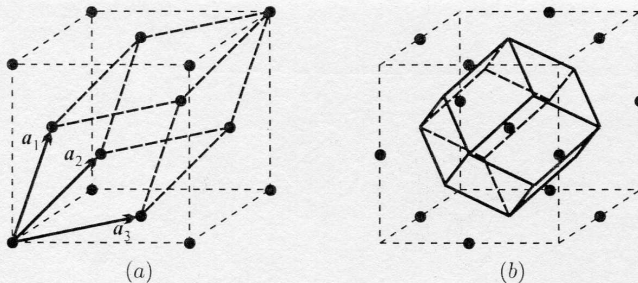
5.27. ábra. Csúsztatva tükrözéssel szemben invariáns atomi elrendeződés



5.28. ábra. Négyfogású csavartengellyel rendelkező atomi elrendeződések. Az egyik esetben jobbra, a másik esetben balra forgatunk, miközben a forgástengely irányában a rácsállandó negyedével eltoljuk a kristályt

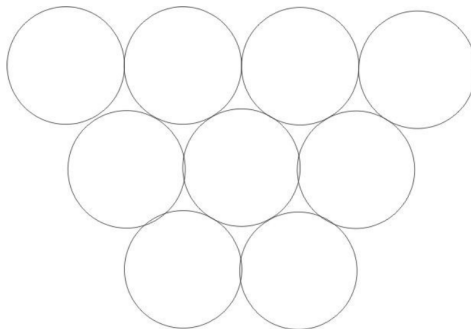


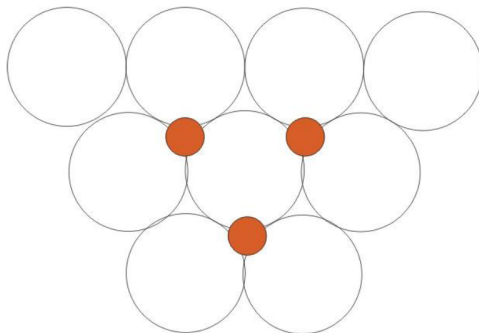
Cr, Fe, Mo, Nb

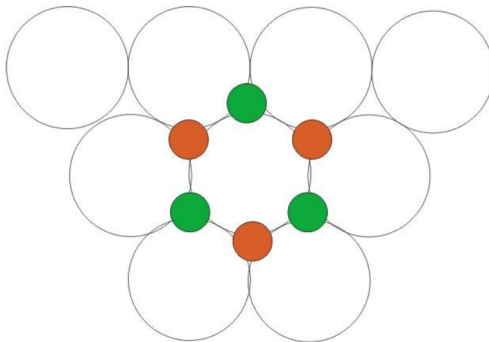


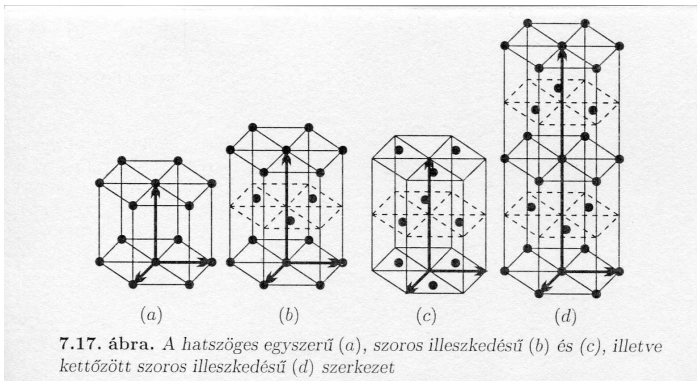
7.9. ábra. Lapcentrált köbös kristály Bravais-cellája az elemi rácsvektorokkal (a) és Wigner-Seitz-cellája (b)

Cu, Ag, Au, Ni

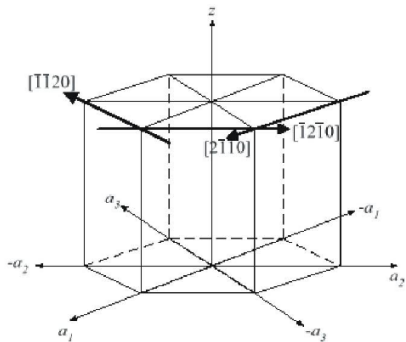


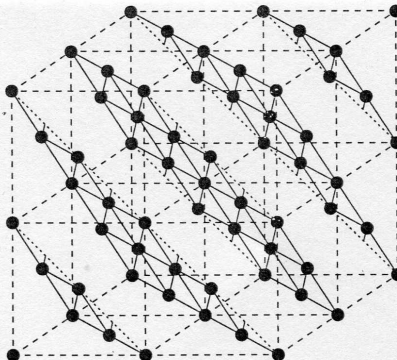




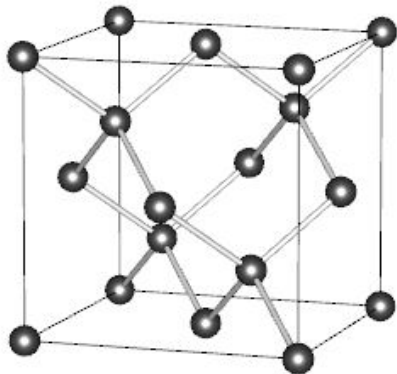
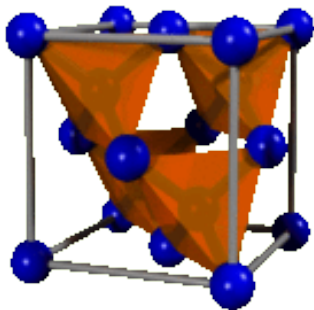


Co, Ti, Zn, Ni, Mg

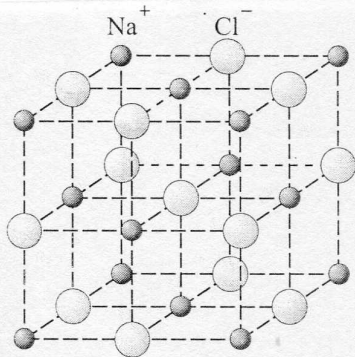




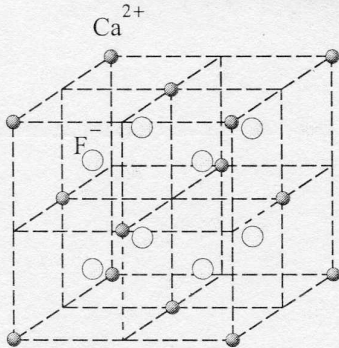
7.11. ábra. Az atomok szoros illeszkedésű elhelyezkedése lapcentrált köbös kristályban a térátlóra merőleges síkokban



FCC eltolása negyed testátlóval



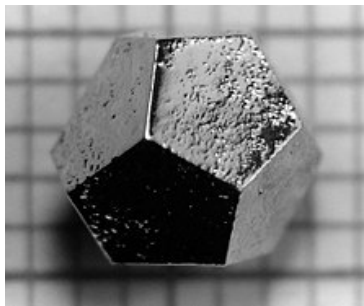
(a)



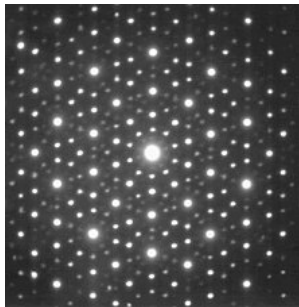
(b)

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

Daniel Dan Shechtman (1982), Nobel díj 2011



Kvázikristály



Diffrakciós kép

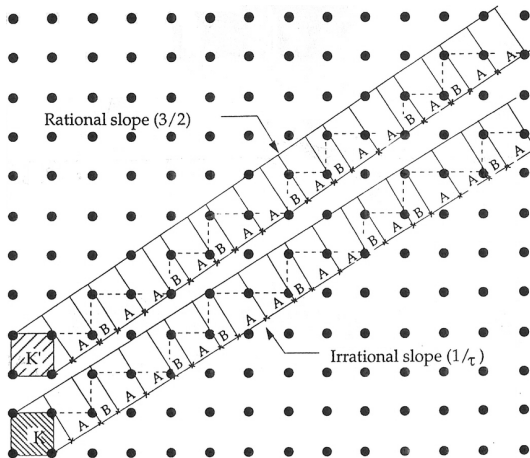
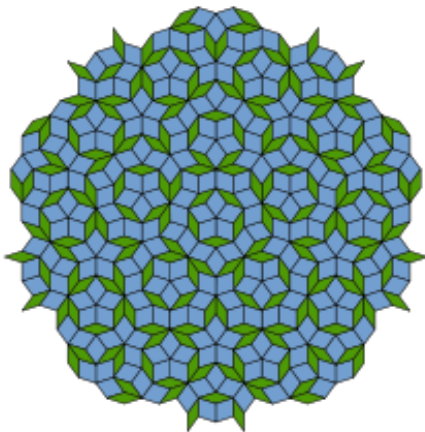


Table 4. The Fibonacci chain.

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	LSLLSLSLSLS	8	5
21	LSLLSLSLSLSLSLSL	13	8
...



Penrose tiling

A kövér rombusznak 72, 72, 108, 108 szögek

A sovány rombusznak 36, 36, 144, 144 szögek