

ELTE III.Fizika BSC

2014/2015 I.félév

Kondenzált anyag fizika

8. GYAKORLAT

(2014. November 4.)

Reciprok rács, Brillouin zóna

Reciprok rács a \underline{b}_j vektorok alkotta rács.

$\underline{K}(\underline{b}_1, \underline{b}_2, \underline{b}_3)$ reciprok rács vektor!

$\underline{K}(2\pi/\underline{a}_1, 2\pi/\underline{a}_2, 2\pi/\underline{a}_3)$

A reciprok rács:

- Valódi rács véges.
- A reciprok rács végtelen.
- A két rács rácspontjai **között nincs** megfeleltetés.
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$$\underline{b}_x = 2\pi \frac{\underline{a}_y \times \underline{a}_z}{V_o}; \underline{b}_y = 2\pi \frac{\underline{a}_z \times \underline{a}_x}{V_o}; \underline{b}_z = 2\pi \frac{\underline{a}_x \times \underline{a}_y}{V_o}$$
$$V_o = (\underline{a}_x \times \underline{a}_y) \cdot \underline{a}_z$$

A reciprokrács elemi cellája (Wigner-Seitz cellája) a Brillouin zóna.

$$V_{\text{Brillouin}} = (\underline{b}_x \times \underline{b}_y) \cdot \underline{b}_z = 8\pi^3 / V_o$$

FCC rács és reciprokrácsa

$$\underline{\mathbf{a}}_1 = \frac{1}{2} a (0,1,1)$$

$$\underline{\mathbf{a}}_2 = \frac{1}{2} a (1,0,1)$$

$$\underline{\mathbf{a}}_3 = \frac{1}{2} a (1,1,0)$$

$$V_0 = a^3/4$$

$$\underline{\mathbf{b}}_1 = (2\pi/a) (2) (1/2) (-1, 1, 1)$$

$$\underline{\mathbf{b}}_2 = (2\pi/a) (2) (1/2) (1, -1, 1)$$

$$\underline{\mathbf{b}}_3 = (2\pi/a) (2) (1/2) (1, 1, -1)$$

$$V_B = (2\pi/a)^3 (2^3) / 2$$

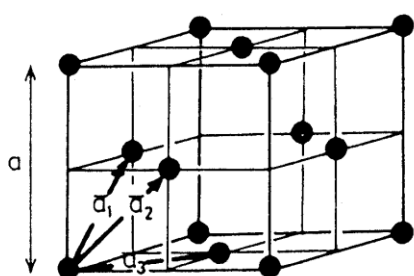
Brillouin zóna = reciprokrács Wigner-Seitz cella

Beírható gömb sugara

$$r = a \sqrt{2} / 4$$

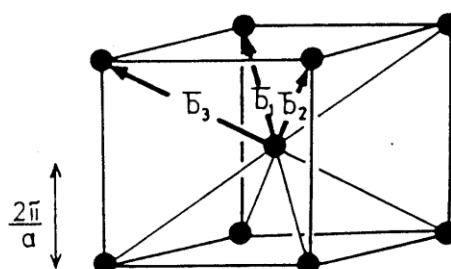
$$k_F = (2\pi/a) \sqrt{3} / 2$$

rács

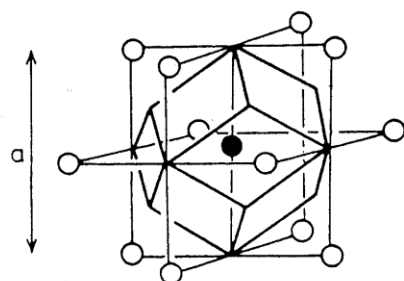


FCC

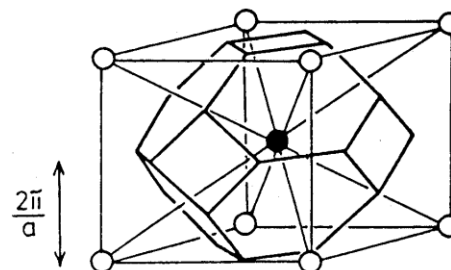
reciprok rács



Wigner-Seitz cella



Brillouin zóna



BCC rács és reciprokrácsa

$$\mathbf{a}_1 = \frac{1}{2} a (-1, 1, 1)$$

$$\mathbf{a}_2 = \frac{1}{2} a (1, -1, 1)$$

$$\mathbf{a}_3 = \frac{1}{2} a (1, 1, -1)$$

$$V_0 = a^3 / 2$$

$$\mathbf{b}_1 = (2\pi/a) (2) (1/2) (0, 1, 1)$$

$$\mathbf{b}_2 = (2\pi/a) (2) (1/2) (1, 0, 1)$$

$$\mathbf{b}_3 = (2\pi/a) (2) (1/2) (1, 1, 0)$$

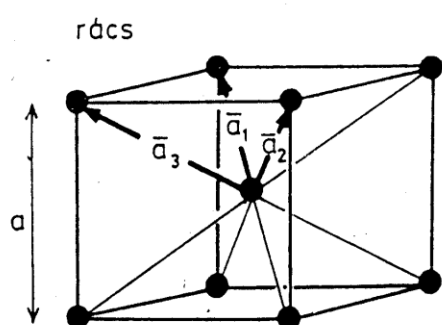
$$V_B = (2\pi/a)^3 (2^3) / 4$$

Brillouin zóna = reciprokrács Wigner-Seitz cella

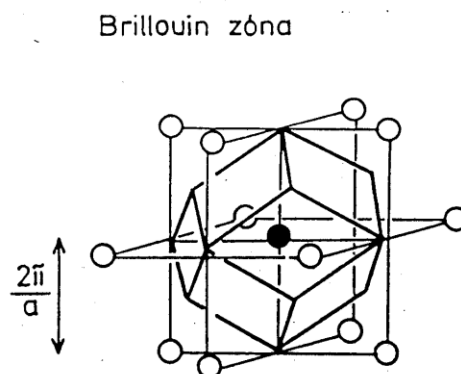
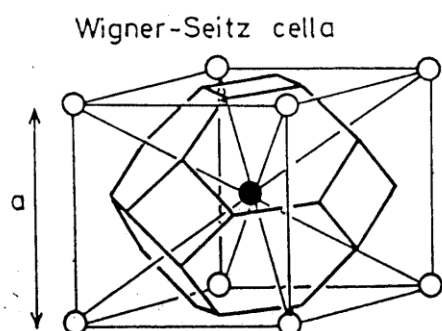
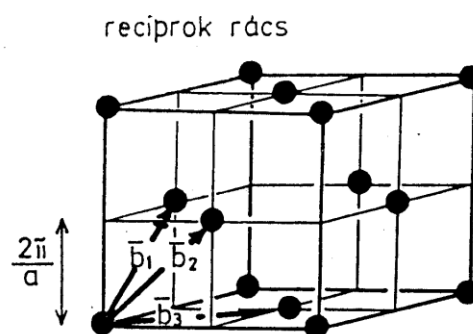
Beírható gömb sugara:

$$r = a \sqrt{3} / 4$$

$$k_F = (2\pi/a) \sqrt{2} / 2$$



BCC



Szoros illeszkedésű hatszöges (HCP) rács és reciprokrácsa

$$\underline{a}_1 = a (1, 0, 0)$$

$$\underline{a}_2 = \frac{1}{2} a (1, \sqrt{3}, 0)$$

$$\underline{a}_3 = c (0, 0, 1)$$

$$V_0 = a^2 c \sqrt{3} / 2$$

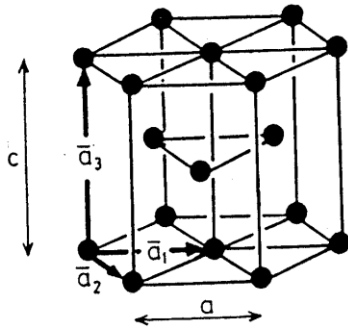
$$\underline{b}_1 = (2\pi/a)(1/\sqrt{3})(\sqrt{3}, -1, 0)$$

$$\underline{b}_2 = (2\pi/a)(2/\sqrt{3})(0, 1, 0)$$

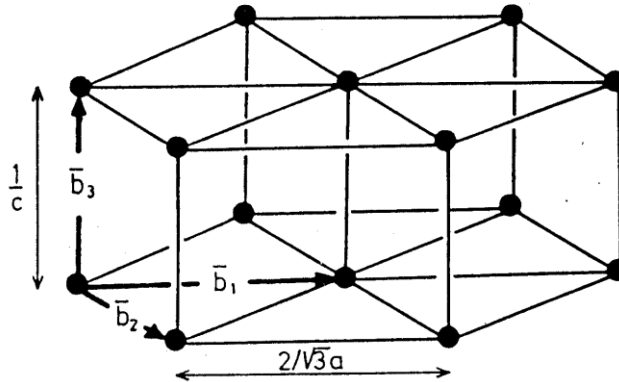
$$\underline{b}_3 = (2\pi/c) (0, 0, 1)$$

$$V_B = (2\pi/a)^2 (2\pi/c) (2/\sqrt{3})$$

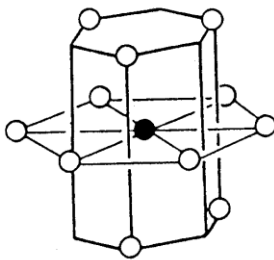
rács



HCP reciprok rács



Wigner-Seitz cella



Brillouin zóna

