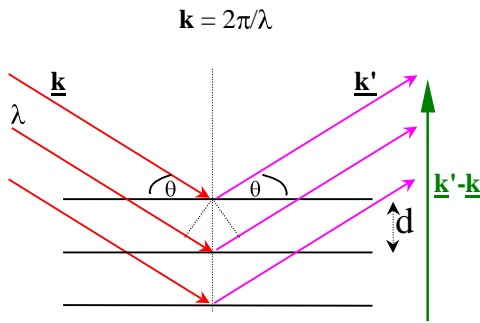


ELTE III.Fizika BSC
2014/2015 I.félév
Kondenzált anyag fizika
 9. GYAKORLAT
 (2014. November 11)

Szerkezetvizsgálatok, diffrakció
Bragg törvény, struktúra faktor



$$k = 2\pi/\lambda$$

$$2d \sin \theta = n \lambda$$

$$(2\pi/\lambda)(2\sin \theta) d = n 2\pi$$

$$\underline{k}' - \underline{k} = h \underline{b}_1 + k \underline{b}_2 + l \underline{b}_3$$

$$e^{i(\underline{k}'-\underline{k})\underline{R}} = 1 \text{ (erősítés)}$$

$$\underline{K} \underline{R} = 2\pi$$

$$\underline{R} = i \underline{a}_1 + j \underline{a}_2 + k \underline{a}_3 \text{ (direkt rács)}$$

$$\underline{K} = h \underline{b}_1 + k \underline{b}_2 + l \underline{b}_3 \text{ (reciprok rács)}$$

Reciprokrács: $\underline{a}_i \underline{b}_j = 2\pi\delta_{ij}$; $\underline{b}_i = 2\pi (\underline{a}_j \times \underline{a}_k)/V_0$; $V_0 = \underline{a}_i (\underline{a}_j \times \underline{a}_k)$
 $V_B = (2\pi)^3/V_0$; $V_B = \underline{b}_i (\underline{b}_j \times \underline{b}_k)$

Polikristályos egyszerű köbös (SC) anyagban a Bragg törvény:

$$(\underline{k}' - \underline{k})^2 = (h \underline{b}_1 + k \underline{b}_2 + l \underline{b}_3)^2 \quad \underline{b}_1 = (2\pi/a) (1,0,0) ; \dots$$

$$(2a \sin \theta / \lambda)^2 = (h^2 + k^2 + l^2)$$

| | | | | | | | | | |
|--------------------------------|---|---|---|---|---|---|---|---|---|
| h | 0 | 1 | 1 | 1 | 2 | 2 | 2 | 2 | 2 |
| k | 0 | 0 | 1 | 1 | 0 | 1 | 1 | 2 | 2 |
| l | 0 | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 1 |
| $(2a \sin \theta / \lambda)^2$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 8 | 9 |

$$(2a \sin \theta / \lambda)^2 = 0, 1, 2, 3, \dots \quad /7, 15, 23, \dots \text{ hiányzik/}$$

Polikristályos FCC anyagban a Bragg törvény:

$$\underline{b}_1 = (2\pi/a) (-1,1,1) ; \underline{b}_2 = (2\pi/a) (1, -1, 1) ; \underline{b}_3 = (2\pi/a) (1, 1, -1)$$

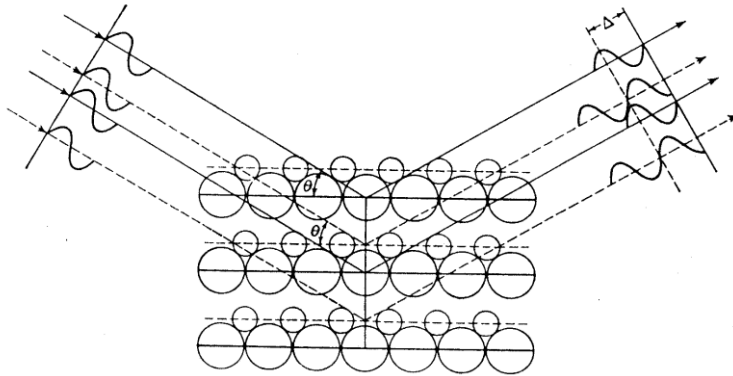
$$(2a \sin \theta / \lambda)^2 = 3(h^2 + k^2 + l^2) - 2(hk + hl + kl)$$

| | | | | | | | | | |
|--------------------------------|---|---|---|---|----|----|---|----|----|
| h | 0 | 1 | 1 | 1 | 2 | 2 | 2 | 2 | 2 |
| k | 0 | 0 | 1 | 1 | 0 | 1 | 1 | 2 | 2 |
| l | 0 | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 1 |
| $(2a \sin \theta / \lambda)^2$ | 0 | 3 | 4 | 3 | 12 | 11 | 8 | 16 | 11 |

$$(2a \sin \theta / \lambda)^2 = 0, 3, 4, 8, 11, 12, 16, \dots$$

Struktúra faktor

Összetett rácsokra egyszerűsítés



$$F_{hkl} = \sum_{n=1}^{\text{cellán belül}} f_n e^{2\pi i (h \frac{a_n}{a} x + k \frac{a_n}{a} y + l \frac{a_n}{a} z)}$$

a) BCC = két egymásba tolt egyszerű köbös rács (SC)

$$\underline{a} = \underline{a}_1 = a (0, 0, 0) \quad ; \quad \underline{a}' = \underline{a}_2 = a/2 (1, 1, 1)$$

$$F_{hkl}^{BCC} = f (1 + e^{\pi i (h+k+l)})$$

$$I \sim F^2$$

$$I \sim 4f^2 \quad \text{ha } h+k+l \text{ páros}$$

$$I \sim 0 \quad \text{ha } h+k+l \text{ páratlan}$$

| | | | | | | | | | | |
|--------------------------------|---|---|---|---|---|----|----|----|----|----|
| h | 0 | 1 | 2 | 2 | 2 | 3 | 2 | 3 | 4 | 4 |
| k | 0 | 1 | 0 | 1 | 2 | 1 | 2 | 2 | 0 | 1 |
| l | 0 | 0 | 0 | 1 | 0 | 0 | 2 | 1 | 0 | 1 |
| $(2a \sin \theta / \lambda)^2$ | 0 | 2 | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 |

$$(2a \sin \theta / \lambda)^2 = 0, 1, 2, 3, \dots, 6, 7, 8, \dots \quad \text{/de 7 nem hiányzik !/}$$

b) FCC = négy egymásba tolt egyszerű köbös rács (SC)

$$\underline{a} = a/2 (0, 0, 0) ; \underline{a}' = a/2 (0, 1, 1) ; \underline{a}'' = a (1, 0, 1) ; \underline{a}''' = a/2 (1, 1, 0)$$

$$F_{hkl}^{FCC} = f (1 + e^{\pi i (k+l)} + e^{\pi i (h+l)} + e^{\pi i (h+k)})$$

$$I \sim F^2$$

$$I \sim 16f^2 \quad \text{ha } h, k, l \text{ azonos paritású}$$

$$I \sim 0 \quad \text{ha } h, k, l \text{ eltérő paritású}$$

| | | | | | | | | | |
|--------------------------------|---|---|---|---|----|----|----|----|----|
| h | 0 | 1 | 2 | 2 | 3 | 2 | 4 | 3 | 4 |
| k | 0 | 1 | 0 | 2 | 1 | 2 | 0 | 3 | 2 |
| l | 0 | 1 | 0 | 0 | 1 | 2 | 0 | 1 | 0 |
| $(2a \sin \theta / \lambda)^2$ | 0 | 3 | 4 | 8 | 11 | 12 | 16 | 19 | 20 |

$$(2a \sin \theta / \lambda)^2 = (h^2 + k^2 + l^2) = 0, 3, 4, 8, 11, 12, 16, \dots \quad (3, 1, 4 \text{ diff.})$$