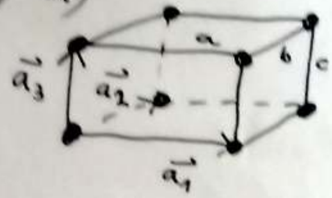
1) a)



$\vec{a}_1 = a(1,0,0)$ $\quad \vec{A}_1 = \frac{2\pi}{a}(1,0,0)$

$\vec{a}_2 = b(0,1,0)$ $\quad \vec{A}_2 = \frac{2\pi}{b}(0,1,0)$ $\quad \vec{a}_i \cdot \vec{A}_j = 2\pi \delta_{ij}$ 1/4

$\vec{a}_3 = c(0,0,1)$ $\quad \vec{A}_3 = \frac{2\pi}{c}(0,0,1)$

↑ koordinatni sistem izberem tako, da je $a > b > c$

b) $\vartheta_1 = 73.74°$, $\vartheta_2 = 97.18°$, $\vartheta_3 = 118.00°$, $\vartheta_4 = 147.67°$

$\vec{K} = 2\pi\left(\frac{m_1}{a}, \frac{m_2}{b}, \frac{m_3}{c}\right) \rightarrow d = \frac{2\pi}{|\vec{K}|} = \frac{1}{\sqrt{\left(\frac{m_1}{a}\right)^2 + \left(\frac{m_2}{b}\right)^2 + \left(\frac{m_3}{c}\right)^2}}$; $2d\sin\frac{\vartheta}{2} = \lambda$

$(100) \rightarrow d_{100} = a = \frac{\lambda}{2\sin\vartheta_1/2} = \underline{\underline{5.00 Å}}$

$(200) \rightarrow d_{200} = \frac{a}{2} < \frac{\lambda}{2}$ ni odboja

$(010) \rightarrow d_{010} = b = \frac{\lambda}{2\sin\vartheta_2/2} = \underline{\underline{4.00 Å}}$

$(110) \rightarrow d_{110} = \frac{1}{\sqrt{\left(\frac{1}{a}\right)^2 + \left(\frac{1}{b}\right)^2}} \rightarrow \vartheta = 2\arcsin\left(\frac{\lambda}{2d_{110}}\right) = \vartheta_4$

$(001) \rightarrow d_{001} = c = \frac{\lambda}{2\sin\vartheta_3/2} = \underline{\underline{3.50 Å}}$ 1/2⁻

c) $\vartheta_1 = 38.94°$, $\vartheta_2 = 83.62°$, $\vartheta_3 = 100.57°$, $\vartheta_4 = 112.89°$, $\vartheta_5 = 113.93°$, $\vartheta_6 = 127.67°$, $\vartheta_7 = 180.00°$

$(100) \rightarrow d_{100} = a = \frac{\lambda}{2\sin\vartheta_1/2} = \underline{\underline{9.00 Å}}$

$(200) \rightarrow d_{200} = \frac{a}{2} \rightarrow \vartheta = 2\arcsin\left(\frac{\lambda}{2d_{200}}\right) = \vartheta_2$

$(300) \rightarrow d_{300} = \frac{a}{3} \rightarrow \vartheta = 2\arcsin\left(\frac{\lambda}{2d_{300}}\right) = \vartheta_7$

$(010) \rightarrow d_{010} = b = \frac{\lambda}{2\sin\vartheta_3/2} = \underline{\underline{3.9 Å}}$

$(110) \rightarrow d_{110} = \frac{1}{\sqrt{\left(\frac{1}{a}\right)^2 + \left(\frac{1}{b}\right)^2}} \rightarrow \vartheta = 2\arcsin\left(\frac{\lambda}{2d_{110}}\right) = \vartheta_5$

$(020), (210) \rightarrow d < \frac{\lambda}{2}$ ni odboja

$(001) \rightarrow d_{001} = c = \frac{\lambda}{2\sin\vartheta_4/2} = \underline{\underline{3.6 Å}}$

$(101) \rightarrow d_{101} = \frac{1}{\sqrt{\left(\frac{1}{a}\right)^2 + \left(\frac{1}{b}\right)^2}} \rightarrow \vartheta = 2\arcsin\left(\frac{\lambda}{2d_{101}}\right) = \vartheta_6$ 1/4⁺

① d) $\vartheta_1 = 34.92°$, $\vartheta_2 = 73.74°$, $\vartheta_3 = 97.18°$, $\vartheta_4 = 107.76°$, $\vartheta_5 = 118.00°$, $\vartheta_6 = 128.32°$, $\vartheta_7 = 130.50°$, $\vartheta_8 = 147.67°$

$(100) \rightarrow d_{100} = \tilde{a} = \frac{\lambda}{2\sin \vartheta_1/2} = 10.00\,\text{Å} = 2a$

Vrhovom pri ϑ_2, ϑ_3, ϑ_5 in ϑ_8 pripišem Millerjeve indekse (200), (010), (001) in (210)

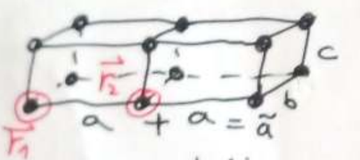
Ostali novi vrhovi so:

$(300) \rightarrow d_{300} = \frac{\tilde{a}}{3} \rightarrow \vartheta = 2\arcsin\left(\frac{\lambda}{2d_{300}}\right) = \vartheta_6$

$(110) \rightarrow d_{110} = \frac{1}{\sqrt{\left(\frac{1}{\tilde{a}}\right)^2 + \left(\frac{1}{b}\right)^2}} \rightarrow \vartheta = 2\arcsin\left(\frac{\lambda}{2d_{110}}\right) = \vartheta_4$

$(101) \rightarrow d_{101} = \frac{1}{\sqrt{\left(\frac{1}{\tilde{a}}\right)^2 + \left(\frac{1}{c}\right)^2}} \rightarrow \vartheta = 2\arcsin\left(\frac{\lambda}{2d_{101}}\right) = \vartheta_7$

Vrednosti sipalnih kotov torej lahko pojasnim s podvojitvijo osnovne celice:



Če bi gradniki ostali na enakih položajih kot pri točki b), bi bila intenziteta novih vrhov enaka nič. Zato se mora en od gradnikov premakniti iz točke Bravaisove mreže:

$\vec{r}_1 = 0$

$\vec{r}_2 = (a + x,\, y,\, z)$

$S_{\vec{k}} = 1 + e^{-i\vec{k}\cdot\vec{r}_2} = 1 + e^{-i\left[\pi m_1 + \frac{2\pi x}{\tilde{a}} m_1 + \frac{2\pi y}{b} m_2 + \frac{2\pi z}{c} m_3\right]}$

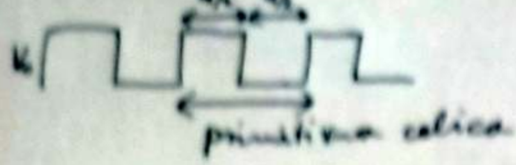
Pri novih vrhovih je m_1 lih, $S_{\vec{k}} = 1 - e^{-2\pi i\left(\frac{x}{\tilde{a}} m_1 + \frac{y}{b} m_2 + \frac{z}{c} m_3\right)}$

$$|S_{\vec{k}}|^2 = 4\sin^2 \pi\left(\frac{x}{\tilde{a}} m_1 + \frac{y}{b} m_2 + \frac{z}{c} m_3\right)$$

Nastanek dodatnih vrhov bi torej lahko bil posledica premika vsake druge mrežne ravnine (100) za majhen x v smeri pravokotno na te ravnine.

1/2

② a)



recipročna mreža: $\frac{2\pi}{a}m$; $m \in \mathbb{Z}$

1. Brillouinova cona: $\left(-\frac{\pi}{a}, \frac{\pi}{a}\right]$

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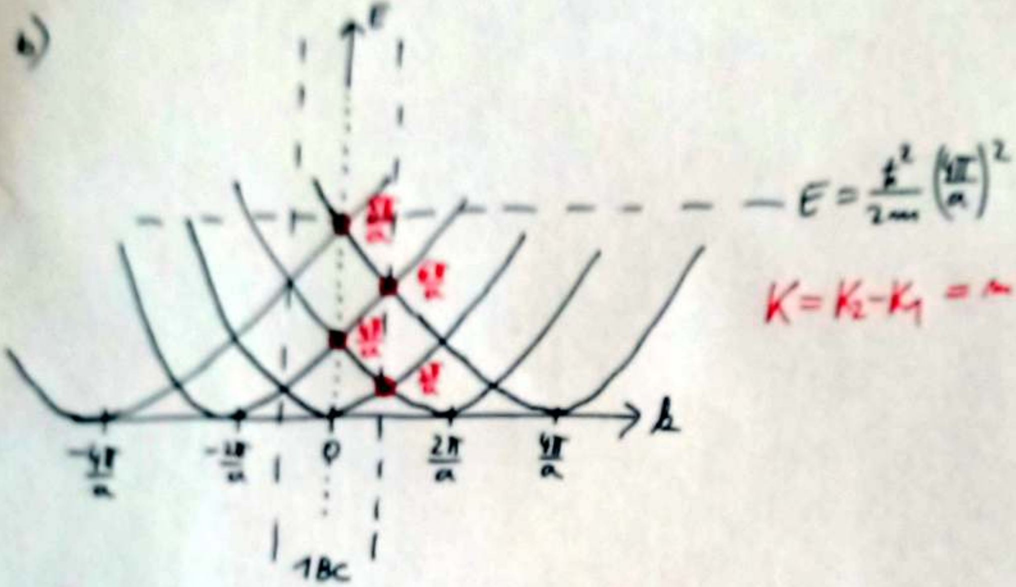
b)



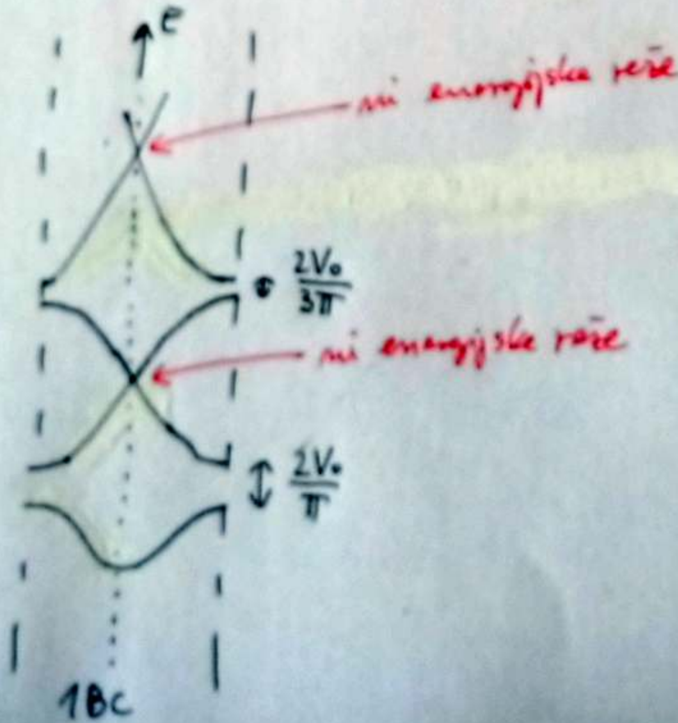
$$m\neq 0:\quad V_K = \frac{1}{a}\int_0^{a/2} V_0 e^{-iKx}\,dx = \frac{V_0}{a}\,\frac{e^{-iKx}}{-iK}\Bigg|_0^{a/2} = \frac{V_0}{-iKa}\left(e^{-iK\frac{a}{2}}-1\right) =$$

$$= \frac{V_0}{-i\frac{2\pi}{a}m\,a}\left[e^{-i\frac{2\pi}{a}m\frac{a}{2}}-1\right] = \frac{V_0}{-2\pi i m}\left[e^{-i\pi m}-1\right] = \begin{cases} 0; & m \text{ sod} \\ \frac{V_0}{i\pi m}; & m \text{ lih} \end{cases}$$

širina energijskih rež: $\Delta E_m = 2\left|V_{m\frac{2\pi}{a}}\right| = \begin{cases} 0; & m \text{ sod} \\ \frac{2V_0}{m\pi}; & m \text{ lih} \end{cases}$

1/2

c)



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