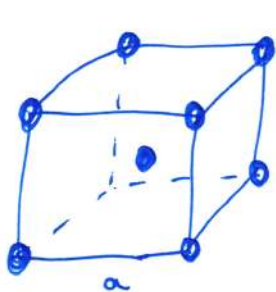


①



$$\begin{aligned}\vec{a}_1 &= a(1, 0, 0) \rightarrow \vec{A}_1 = \frac{2\pi}{a}(1, 0, 0) \\ \vec{a}_2 &= a(0, 1, 0) \rightarrow \vec{A}_2 = \frac{2\pi}{a}(0, 1, 0) \\ \vec{a}_3 &= a(0, 0, 1) \rightarrow \vec{A}_3 = \frac{2\pi}{a}(0, 0, 1)\end{aligned}$$

$$\begin{aligned}\vec{r}_1 &= 0 \\ \vec{r}_2 &= a\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)\end{aligned}$$

$$S_{\vec{k}} = 1 + e^{-i\vec{k} \cdot \vec{r}_2} \quad \vec{k} = \frac{2\pi}{a}(m_1, m_2, m_3)$$

$$S_{\vec{k}} = 1 + e^{-i\pi(m_1 + m_2 + m_3)} = \begin{cases} 2; & m_1 + m_2 + m_3 \text{ lih} \\ 0; & m_1 + m_2 + m_3 \text{ liho} \end{cases}$$

a) $2d \sin \frac{\theta}{2} = \lambda$

$$d = \frac{2\pi}{|\vec{k}|} = \frac{a}{\sqrt{m_1^2 + m_2^2 + m_3^2}}$$

$$\left. \begin{aligned} \sin \frac{\theta}{2} &= \frac{\lambda}{2a} \sqrt{m_1^2 + m_2^2 + m_3^2} \\ a &= 4\text{\AA}, \lambda = 3\text{\AA} \Rightarrow m_1^2 + m_2^2 + m_3^2 \leq 7 \end{aligned} \right\}$$

$$a = 4\text{\AA}, \lambda = 3\text{\AA} \Rightarrow m_1^2 + m_2^2 + m_3^2 \leq 7$$

$\{100\}$ $m_1 + m_2 + m_3$ lih

$\{110\} \Rightarrow \theta_1 = 64.1^\circ$

$\{111\}$ $m_1 + m_2 + m_3$ liho

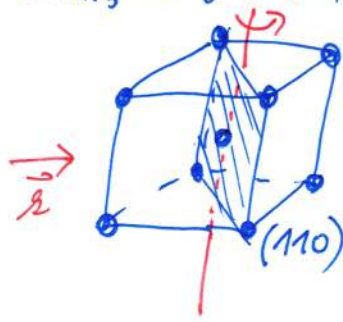
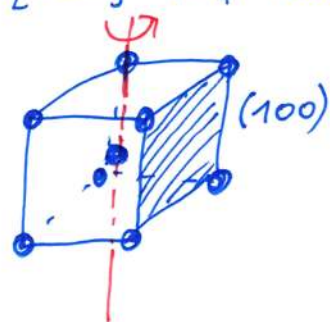
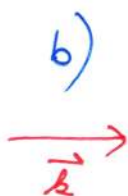
$\{200\} \Rightarrow \theta_2 = 97.1^\circ$

$\{210\}$ $m_1 + m_2 + m_3$ lih

$\{211\} \Rightarrow \theta_3 = 133.4^\circ$

$\{220\}$ $m_1^2 + m_2^2 + m_3^2 = 8 > 7.1$

3/4-



Pri rotaciji monokristala kot med $\vec{k}$ in pravokotnico na ravnini (100) in (110) zavzame vse vrednosti med 0° in 90° , zato bomo Braggova odboja na teh ravninah pri kotih 64.1° in 97.1° opazili.

Poglejmo še odboje na ravninah $\{211\}$:

$$\vec{k} - \vec{k}' = \vec{K} \rightarrow \vec{k} \cdot \vec{K} = \frac{K^2}{2}$$



$$2 = |\vec{k}| = |\vec{k}'| = \frac{2\pi}{\lambda}$$

$$(2x, 2y, 0) \cdot \frac{2\pi}{a}(m_1, m_2, m_3) = \left(\frac{2\pi}{a}\right)^2 (m_1^2 + m_2^2 + m_3^2)$$

$$m_1 2x + m_2 2y = \frac{1}{2} \frac{2\pi}{a} (m_1^2 + m_2^2 + m_3^2)$$

$$m_1 \cos \alpha + m_2 \sin \alpha = \frac{\lambda}{2a} (m_1^2 + m_2^2 + m_3^2)$$

$$2x = \frac{2\pi}{\lambda} \cos \alpha$$

$$2y = \frac{2\pi}{\lambda} \sin \alpha$$

za ravnine $\{211\}$: $m_1 \cos \alpha + m_2 \sin \alpha = \frac{\lambda}{2a} 6 = \frac{9}{4}$

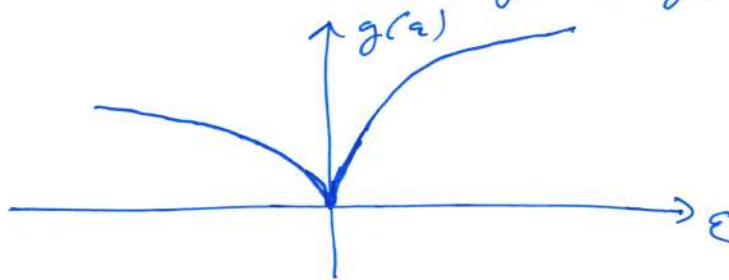
Braggov odboj: bomo opazili, če obstaja zasuk kristala α , ki reši to enačbo. Ker je $\frac{9}{4} > 2$, mora biti $m_1 = 2$ in $m_2 = 1$ (ali obratno):

$$2 \cos \alpha + 1 \sin \alpha = \operatorname{Re}\{2e^{i\alpha} - i e^{i\alpha}\} = \operatorname{Re}\{\sqrt{5} e^{i(\alpha + \delta)}\} \leq \sqrt{5} < \frac{9}{4} \quad 1/4^+$$

Braggovega odboja pri kotu 133.4° torej ne opazimo.

(2) a) $\epsilon_2(\vec{k}) = \frac{\hbar^2 k^2}{2m_2} \rightarrow g_2(\epsilon) = \frac{\sqrt{2m_2^3}}{\pi^2 \hbar^3} \sqrt{\epsilon} \theta(\epsilon)$ iz vaj
 $\epsilon_1(\vec{k}) = -\frac{\hbar^2 k^2}{2m_1} \rightarrow g_1(\epsilon) = \frac{\sqrt{2m_1^3}}{\pi^2 \hbar^3} \sqrt{-\epsilon} \theta(-\epsilon)$
 $g(\epsilon) = g_1(\epsilon) + g_2(\epsilon) \quad 1/2^-$

b) $m_2 > m_1 \rightarrow$ za $\epsilon > 0$: $g(\epsilon) \neq g(-\epsilon) \left(\frac{m_2}{m_1}\right)^{3/2} > g(-\epsilon)$



$\mu(T=0K) = 0$ Če bi pri $T > 0K$ μ ostal enak 0, bi se št. elektronov v sistemu povečalo, saj bi bilo št. zasedenih stanj v prevodnem pasu večje od št. nezasedenih stanj v valenčnem pasu. Zato je $\mu(T > 0K) < 0$. 1/4

c) $\frac{E}{V} = \int_{-\infty}^{\infty} d\epsilon \epsilon g(\epsilon) f(\epsilon)$ za $m_1 = m_2$ je $g(-\epsilon) = g(\epsilon)$ in $\mu(T) = 0$.

$$\frac{E}{V} = \int_{-\infty}^0 d\epsilon \epsilon g(\epsilon) + \int_{-\infty}^0 d\epsilon \epsilon g(\epsilon) [f(\epsilon) - 1] + \int_0^{\infty} d\epsilon \epsilon g(\epsilon) f(\epsilon) =$$

$$= \frac{E(T=0K)}{V} + \int_{-\infty}^0 d\epsilon \epsilon g(\epsilon) [-f(-\epsilon)] + \int_0^{\infty} d\epsilon \epsilon g(\epsilon) f(\epsilon)$$

$$\frac{E}{V} - \frac{E(T=0K)}{V} = 2 \int_0^{\infty} d\epsilon \epsilon g(\epsilon) f(\epsilon) \propto \int_0^{\infty} d\epsilon \epsilon \sqrt{\epsilon} f(\epsilon) = \int_0^{\infty} d\epsilon \epsilon \sqrt{\epsilon} \frac{1}{e^{\beta \epsilon} + 1} \propto$$

$$\propto \beta^{-5/2} \propto T^{5/2} \rightarrow C \propto T^{3/2} \quad 1/4^+$$