① Diamant ima diamantno kristalno mrežo, ki je sestavljena iz dveh enakih fcc mrež, zamaknjenih za četrtino telesne diagonale konvencionalne osnovne celice fcc mreže. Obravnavamo ga kot sc mrežo z bazo:

$$\left.\begin{array}{ll} \vec{a_1} = a(1,0,0) & \vec{A_1} = \frac{2\pi}{a}(1,0,0) \\ \vec{a_2} = a(0,1,0) & \vec{A_2} = \frac{2\pi}{a}(0,1,0) \\ \vec{a_3} = a(0,0,1) & \vec{A_3} = \frac{2\pi}{a}(0,0,1) \end{array}\right\} \vec{K} = \frac{2\pi}{a}(m_1, m_2, m_3)$$

$$\vec{r_1} = 0$$
$$\vec{r_2} = a\left(0, \tfrac{1}{2}, \tfrac{1}{2}\right)$$
$$\vec{r_3} = a\left(\tfrac{1}{2}, 0, \tfrac{1}{2}\right)$$
$$\vec{r_4} = a\left(\tfrac{1}{2}, \tfrac{1}{2}, 0\right)$$
$$\vec{r}_{i+4} = \vec{r_i} + \vec{d} \quad \text{za } i = 1,2,3,4, \quad \vec{d} = \frac{a}{4}(1,1,1)$$

$$S_{\vec{K}} = \sum_{i=1}^{8} e^{-i\vec{K}\cdot\vec{r_i}} = \sum_{i=1}^{4} e^{-i\vec{K}\cdot\vec{r_i}}\left(1 + e^{-i\vec{K}\cdot\vec{d}}\right) = S_{\vec{K}}^{fcc}\left(1 + e^{-i\frac{\pi}{2}(m_1+m_2+m_3)}\right)$$

Iz vaj: $S_{\vec{K}}^{fcc} \neq 0$, če so m_1, m_2, m_3 vsi sodi ali vsi lihi.

Dodatno je $1 + e^{-i\frac{\pi}{2}(m_1+m_2+m_3)} = 0$ za $m_1 + m_2 + m_3 = 4N+2$; $N \in \mathbb{Z}$

1/4+

a) $2d\sin\frac{\vartheta}{2} = \lambda$, $d = \frac{2\pi}{|\vec{K}|} = \frac{a}{\sqrt{m_1^2 + m_2^2 + m_3^2}}$

$$\sin\frac{\vartheta}{2} = \frac{\lambda}{2a}\sqrt{m_1^2 + m_2^2 + m_3^2}$$

$$\sin\frac{\vartheta}{2} \leq 1 \longrightarrow m_1^2 + m_2^2 + m_3^2 \leq 21$$

$\lvert m_1 \rvert$	$\lvert m_2 \rvert$	$\lvert m_3 \rvert$	ϑ
1	1	1	43.94°
2	2	0	75.32°
3	1	1	91.52°
4	0	0	119.54°
3	3	1	140.63°

1/4+

b) $\vec{k} = \frac{2\pi}{\lambda}(1,0,0)$ $\quad \vartheta = 180° \rightarrow \vec{K} \parallel \vec{k}$; $\vec{K} = (4N, 0, 0)$, $N \in \mathbb{N}$

$$\lambda = 2d = \frac{2a}{4N}$$

N	λ
1	1.7835 Å
2	0.8918 Å
3	0.5945 Å

1/4+

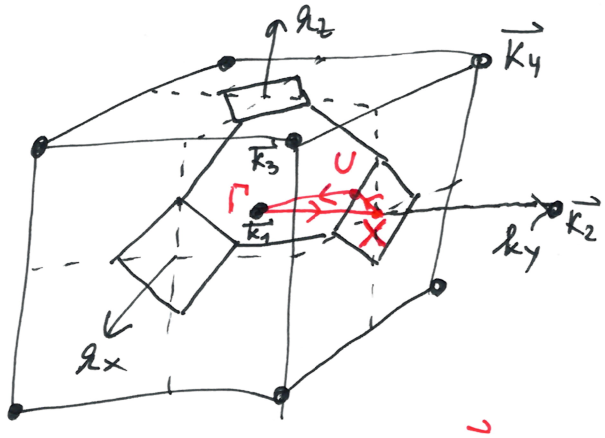
2 a) $\rho = \frac{4m_1}{a^3}$ (4 atomi na konvencionalno osnovno celico, $m_1 = \frac{M}{N_A}$ je masa enega atoma)

$$a = \sqrt[3]{\frac{4M}{\rho N_A}} = \underline{\underline{4.08\ \text{Å}}}$$ 1/4

b) $N = 2 \cdot \frac{\frac{4\pi k_F^3}{3}}{\frac{(2\pi)^3}{V}} \rightarrow \frac{N}{V} = \frac{4}{a^3} = \frac{k_F^3}{3\pi^2} \rightarrow k_F = \frac{(12\pi^2)^{1/3}}{a}$

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2ma^2}(12\pi^2)^{2/3} = \underline{\underline{5.52\,\text{eV}}}$$ 1/4

c)



$\vec{K}_1 = 0 = \Gamma$

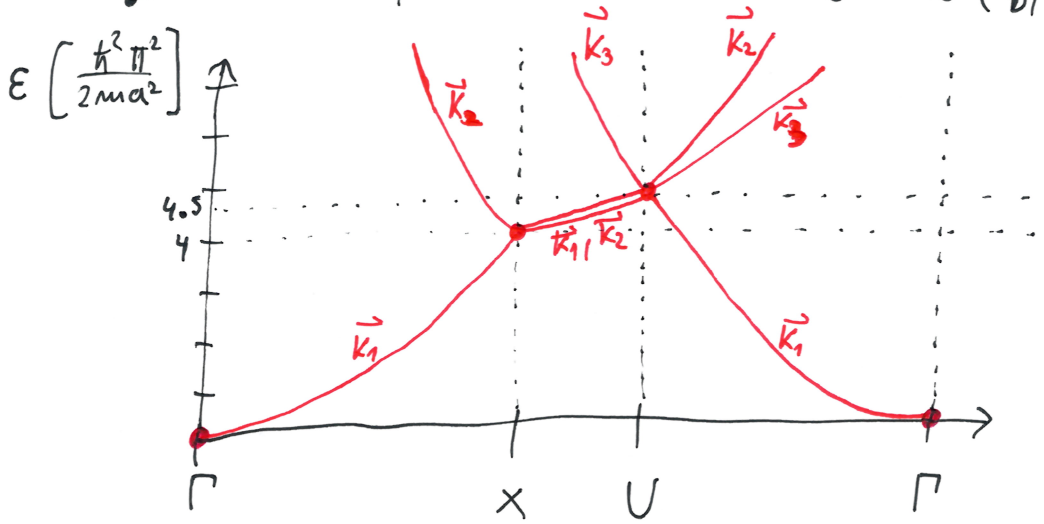
$\vec{K}_2 = \frac{4\pi}{a}(0, 1, 0)$

$\vec{K}_3 = \frac{4\pi}{a}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$

$\vec{K}_4 = \frac{4\pi}{a}\left(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$

$X = \frac{4\pi}{a}\left(0, \frac{1}{2}, 0\right) \qquad |X| = 2\frac{\pi}{a}$

$U = \frac{4\pi}{a}\left(\frac{1}{8}, \frac{1}{2}, \frac{1}{8}\right) \quad |U| = \sqrt{4.5}\,\frac{\pi}{a}$



$|U - \vec{K}_4| = \sqrt{8.5}\,\frac{\pi}{a}$

$|X - \vec{K}_4| = |X - \vec{K}_3| = \sqrt{8}\,\frac{\pi}{a}$

1/4

d) V točki U imamo trojno degeneracijo: $|U - \vec{K}_1| = |U - \vec{K}_2| = |U - \vec{K}_3|$

$$V_{\vec{k}} = \frac{1}{V_{oc}}\int_{oc} V(\vec{r})e^{-i\vec{k}\cdot\vec{r}}d\vec{r} = \frac{1}{\frac{1}{4}a^3}\int_{o.c} -\lambda\delta(\vec{r})e^{-i\vec{k}\cdot\vec{r}}d\vec{r} = -\frac{4\lambda}{a^3} \equiv V$$

$$\begin{vmatrix} \varepsilon^0 + V - \varepsilon, & V, & V \\ V, & \varepsilon^0 + V - \varepsilon, & V \\ V, & V, & \varepsilon^0 + V - \varepsilon \end{vmatrix} = \begin{vmatrix} \varepsilon^0 - \varepsilon, & V, & 0 \\ \varepsilon - \varepsilon^0, & \varepsilon^0 + V - \varepsilon, & \varepsilon - \varepsilon^0 \\ 0, & V, & \varepsilon^0 - \varepsilon \end{vmatrix} = \begin{vmatrix} \varepsilon^0 - \varepsilon, & V, & 0 \\ 0, & \varepsilon^0 + 3V - \varepsilon, & 0 \\ 0, & V, & \varepsilon^0 - \varepsilon \end{vmatrix} =$$

$$(\varepsilon^0 - \varepsilon)^2(\varepsilon^0 + 3V - \varepsilon) = 0$$

$\varepsilon_{1,2} = \varepsilon^0$

$\varepsilon_3 = \varepsilon^0 + 3V \quad , \quad \varepsilon^0 = \frac{\hbar^2}{2m}U^2$ 1/4