① a) **CsCl** SC + baza: $\vec{r}_{Cl^-} = 0$

$$\vec{r}_{Cs^+} = a\left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right)$$

$$S(\vec{k}) = f_{Cl^-}(\vec{k})e^{-i\vec{k}\cdot\vec{r}_{Cl^-}} + f_{Cs^+}(\vec{k})e^{-i\vec{k}\cdot\vec{r}_{Cs^+}}$$

$$\vec{k} = \frac{2\pi}{a}(m_1, m_2, m_3)$$

$$S(\vec{k}) = f_{Cl^-}(\vec{k}) + f_{Cs^+}(\vec{k})e^{-i\pi(m_1+m_2+m_3)}$$

različen od ϕ za $\forall m_1, m_2, m_3$

NaCl Cl^- tvorijo FCC; Na^+ tudi, le da je premaknjena za polovico roba kubične osnovne celice

Strukturni faktor izračunamo podobno kot smo ga na vajah za diamant:

$$S(\vec{k}) = S_{FCC}(\vec{k})\left[f_{Cl^-}(\vec{k}) + f_{Na^+}(\vec{k})e^{-i\vec{k}\cdot\frac{a}{2}(1,0,0)}\right] =$$

$$= S_{FCC}(\vec{k})\left[f_{Cl^-}(\vec{k}) + f_{Na^+}(\vec{k})e^{-i\pi m_1}\right]$$

$\hookrightarrow \neq \phi$ za $\forall m_1, m_2, m_3$

$\downarrow$ geometrijski strukturni faktor za FCC; različen od ϕ, če so m_1, m_2, m_3 vsi sodi ali vsi lihi.

$1/2^-$

b) in c)

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

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

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

	$a(\theta_1)$	$a(\theta_2)$	...
1. vzorec			
CsCl	{100} 4.120 Å	{110} 4.121 Å	1. vzorec je CsCl z $a = 4.12$ Å
NaCl	{111} 3.257 Å	{200} 3.988 Å	
2. vzorec			
CsCl	{100} 7.136 Å	{110} 5.827 Å	
NaCl	{111} 5.641 Å	{200} 5.640 Å	2. vzorec je NaCl z $a = 5.64$ Å

$1/2^+$

② a) $\rho = \frac{4 m_1}{a^3}$ ← masa atoma ; $m_1 = \frac{M}{N_A}$

(4 atomi v kubični osnovni celici)

$$a = \sqrt[3]{\frac{4M}{\rho N_A}} = \underline{\underline{4.05\ \text{Å}}} \quad 1/4$$

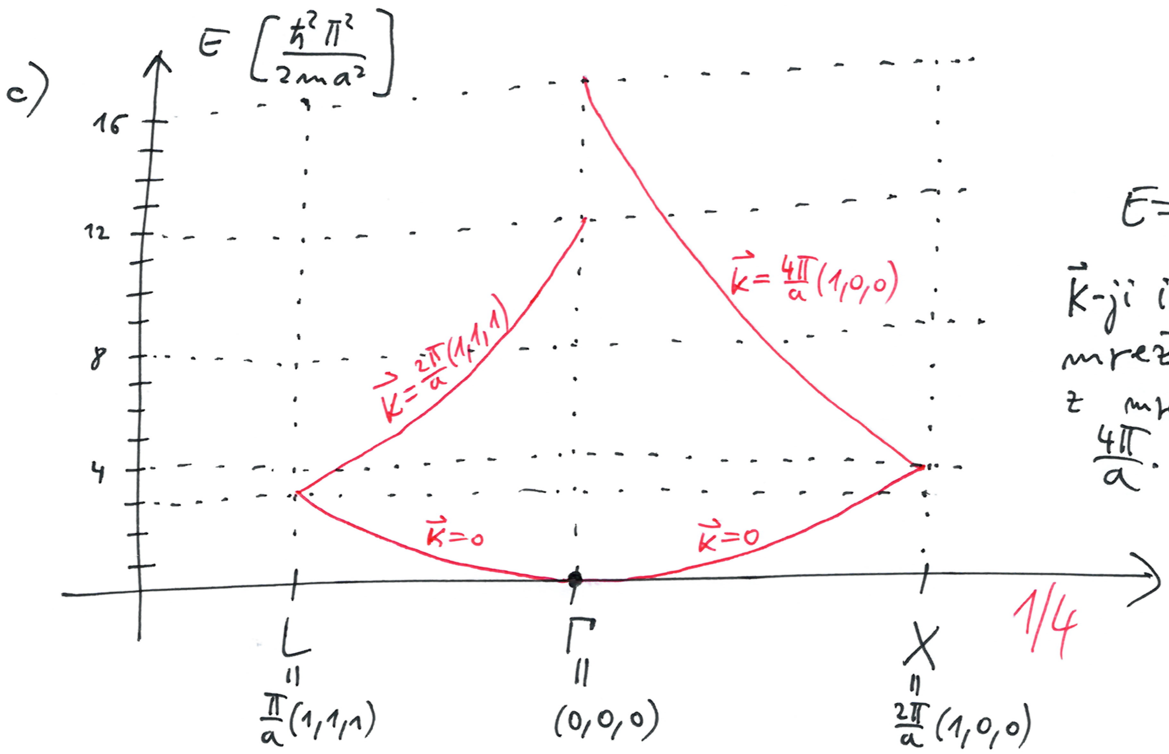
b) $\varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$, $N = \underset{\text{spin}}{2} \frac{V}{(2\pi)^3} \int\limits_{|k|<k_F} d\vec{k} = V \frac{k_F^3}{3\pi^2}$

$$k_F = \sqrt[3]{3\pi^2 \frac{N}{V}} , \quad \frac{N}{V} = \frac{4 \cdot 3}{a^3}$$

(3 valenčni elektroni na atom)

$$\varepsilon_F = \frac{\hbar^2 \pi^2}{2ma^2} \left(\frac{36}{\pi}\right)^{2/3} = \underline{\underline{11.6\ \text{eV}}} \quad 1/4$$

c)



1/4

$$E = \frac{\hbar^2}{2m}(\vec{k} - \vec{K})^2$$

$\vec{K}$-ji iz recipročne mreže, to je BCC z mrežno razdaljo $\frac{4\pi}{a}$.

d) X leži na Braggovi ravnini med $\vec{K}_1 = 0$ in $\vec{K}_2 = \frac{4\pi}{a}(1,0,0)$

L leži na Braggovi ravnini med $\vec{K}_1' = 0$ in $\vec{K}_2' = \frac{2\pi}{a}(1,1,1)$

$$\Delta E = 2\,|V_{\vec{K}_2 - \vec{K}_1}|$$

$$\Delta E' = 2\,|V_{\vec{K}_2' - \vec{K}_1'}|$$

$$V_{\vec{K}} = \frac{1}{V_{o.c.}} \int\limits_{o.c.} V(\vec{r})\, e^{-i\vec{K}\cdot\vec{r}} = \frac{1}{a^3/4} \int\limits_{o.c.} \lambda\, \delta(\vec{r})\, e^{-i\vec{K}\cdot\vec{r}} = \frac{4\lambda}{a^3}$$

$$\underline{\underline{\Delta E = \Delta E' = \frac{8|\lambda|}{a^3}}} \quad 1/4$$