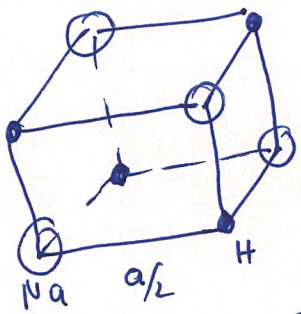
FFY 011 - 2013
Dugga 2013-02-14
Lösningar

1a) NaCl struktur (se Kittel s 13 + 14)



Na: $(000)\ (\tfrac12\tfrac12 0)\ (\tfrac12 0\tfrac12)\ (0\tfrac12\tfrac12)$
H: $(\tfrac12 00)\ (0\tfrac12 0)\ (00\tfrac12)\ (\tfrac12\tfrac12\tfrac12)$

$$S_{hkl} = \sum_{j=1}^{B} f_j e^{-i\vec{G}_{hkl}\cdot\vec{R}_j} \Rightarrow \sum_j f_j e^{-i2\pi(hx_j+ky_j+lz_j)} =$$

$$S_{hkl} = f_{Na}\left(1 + e^{-i\pi(h+k)} + e^{-i\pi(h+l)} + e^{-i\pi(k+l)}\right) +$$
$$+ f_H\left(e^{-i\pi h} + e^{-i\pi k} + e^{-i\pi l} + e^{-i\pi(h+k+l)}\right).$$

$$S_{111} = 4f_{Na} - 4f_H \quad \text{men } -f_H \approx f_{Na} \Rightarrow S_{111} \approx 8f_{Na}$$
$$S_{200} = 4f_{Na} + 4f_H \qquad\qquad S_{200} \approx 0$$

$$\Rightarrow I_{111} \propto |S_{111}|^2 = 64 f_{Na}^2 \Rightarrow \underline{I_{111} \gg I_{200}}$$
$$I_{200} \propto |S_{200}|^2 \approx 0$$

ZnS struktur (se s. 17+18 i Kittel.)

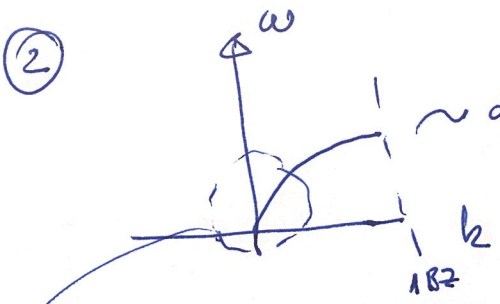
Na: $(000)\ (\tfrac12\tfrac12 0)\ (\tfrac12 0\tfrac12)\ (0\tfrac12\tfrac12)$
H: $(\tfrac14\tfrac14\tfrac14)\ (\tfrac14\tfrac34\tfrac34)\ (\tfrac34\tfrac14\tfrac34)\ (\tfrac34\tfrac34\tfrac14)$

$$S_{hkl} = \sum_j f_j e^{i\vec{G}\cdot\vec{R}_j} = f_{Na}\left(1 + e^{i\pi(k+l)} + e^{-i\pi(h+l)} + e^{-i\pi(h+k)}\right) +$$
$$+ f_H\left(e^{i\frac{\pi}{2}(h+k+l)} + e^{-i\pi/2(h+3k+3l)} + e^{-i\frac{\pi}{2}(3h+k+l)} + e^{-i\frac{\pi}{2}(3h+3k+l)}\right)$$

$$\Rightarrow S_{111} = 4f_{Na} - 4if_H \Rightarrow I_{111} \propto |S_{111}|^2 \propto S\cdot S^* = (4f_{Na})^2 + (4f_H)^2 = 32 f_{Na}^2$$
$$S_{200} = 4f_{Na} - 4f_H \approx 8f_{Na} \Rightarrow I_{200} \approx 64 f_{Na}^2$$

$\Rightarrow$ NaCl strukturen är vanligast pga $I_{111} \gg I_{200}$

(2)



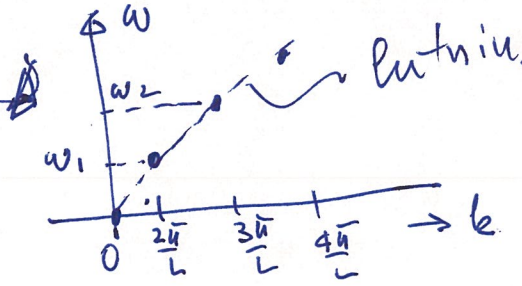
~ dispersion relation $\omega(k)$ för akustiska fononer

$k \in (0 \to$ BZ - kanten)

k diskret; $\quad k = n \cdot \frac{2\pi}{L}$ där $L \equiv$ provets dimension

$n = 0, 1, 2 \ldots$

lägst k-värdet $\equiv k_{min} = \frac{2\pi}{L}$



~ lutningen $\frac{d\omega}{dk} = v$

$$\hbar\omega_1 = \hbar v k_{min} = \hbar v \cdot \frac{2\pi}{L}$$

$$k_B T = \hbar v \frac{2\pi}{L}$$

$$L = \frac{\hbar v \cdot 2\pi}{k_B T} = \frac{1.05 \cdot 10^{-34}\ \text{Js} \cdot 1000\ \text{m/s} \cdot 2\pi}{1.38 \cdot 10^{-23}\ \text{J/k} \cdot 4\ \text{k}} = 1.2 \cdot 10^{-8}\ \text{m} = \underline{120\ \text{Å}}$$

Svar: Provet skall vara cka $L \times L \times L = (120\ \text{Å})^3$

Antalet atomer $\approx \left(\frac{L}{a}\right)^3 = (40)^3 = 64000$