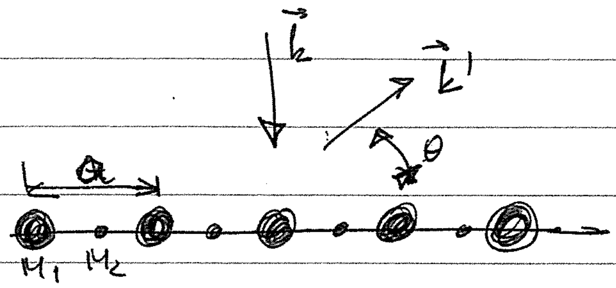
Dugga 110210

Lösningar:

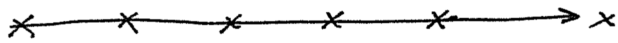
1 a)

Kristall:



Kristall = gitter + bas

gitter:

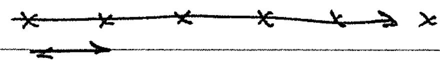


bas:

basvektorer $\vec{r}_1 = \vec{r}_{Cl} = 0$

$r_2 = r_{Na} = \frac{1}{2} a \hat{x}$

Reciproka gittret:



Transl. vektorer i rec. rummet: $\vec{G}_h = h \cdot \frac{2\pi}{a} \hat{x} \quad h = 0, 1, 2, 3$

Diffraktion:

Laue villkor: $\vec{\Delta k} = \vec{G}$

$$\vec{k} - \vec{k}' = h \cdot \frac{2\pi}{a} \hat{x}$$

multiplicera med $\hat{x}$ $\Rightarrow$

$$(\vec{k} - \vec{k}') \cdot \hat{x} = h \cdot \frac{2\pi}{a} \hat{x} \cdot \hat{x}$$

men $\vec{k} \cdot \hat{x} = 0$ pga $\vec{k} \perp \hat{x}$

$$-\vec{k}' \cdot \hat{x} = h \cdot \frac{2\pi}{a}$$

$$\Rightarrow \quad \frac{2\pi}{\lambda} \cdot \cos\theta = h \cdot \frac{2\pi}{a}$$

$$\boxed{h \cdot \lambda = a \cos\theta}$$

$h = 0 \Rightarrow \cos\theta_0 = 0 \Rightarrow \theta_0 = \frac{\pi}{2} \Rightarrow \underline{\theta_0 = 90^\circ}$

$h = 1 \Rightarrow \cos\theta_1 = \frac{2.4}{5.64} = 0.43 \Rightarrow \underline{\theta_1 = 64{,}82^\circ}$

$h = 2 \Rightarrow \cos\theta_2 = \frac{4.8}{5.64} = 0.85 \Rightarrow \underline{\theta_2 = 31.67^\circ}$

(1b) $F = N \cdot S \cdot GS$

om $\Delta\vec{k} = \vec{G} \Rightarrow GS = 1$ och

$$F = N \cdot S$$

där $S = \sum_{\text{atomer i basen}} f_j e^{i\vec{G}\cdot\vec{r}_j}$

Vi har: $\vec{G} = h \cdot \frac{2\pi}{a}\hat{x}$, $\vec{r}_{Cl} = 0$ och $\vec{r}_{Na} = \frac{1}{2}a\hat{x} \Rightarrow$

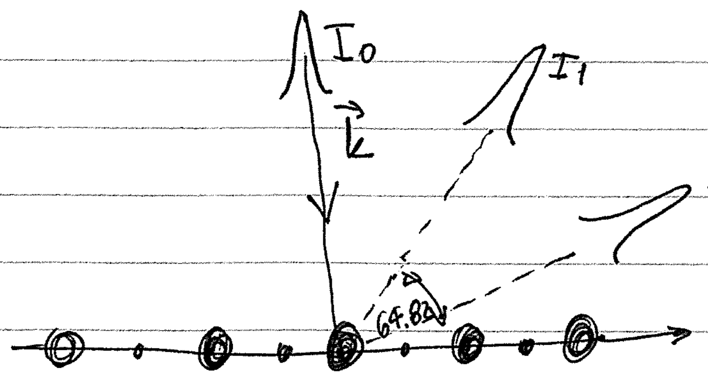
$$F = N \cdot \left(f_{Cl} e^{i\vec{G}\cdot\vec{0}} + f_{Na} e^{i h \frac{2\pi}{a}\hat{x} \cdot \frac{1}{2}a\hat{x}} \right)$$

$$F = N\left(f_{Cl} + f_{Na} e^{ih\pi} \right) \text{ där } h = 0, 1, 2, \ldots$$

om $h = 0 \Rightarrow F_0 = N(f_{Cl} + f_{Na}) \Rightarrow I_0 = N^2 (f_{Na} + f_{Cl})^2$

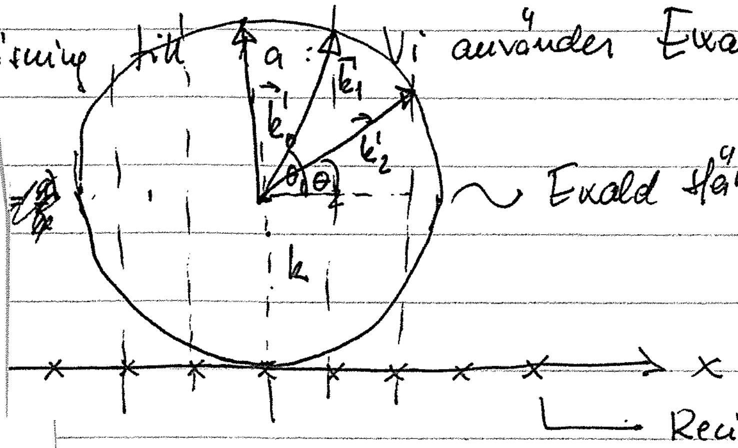
$h = 1 \Rightarrow F_1 = N(f_{Cl} - f_{Na}) \Rightarrow I_1 = N^2 (f_{Cl} - f_{Na})^2$

$h = 2 \Rightarrow F_2 = N(f_{Cl} + f_{Na}) \Rightarrow I_2 = N^2 (f_{Cl} + f_{Na})^2$



Vi har symmetrisk fördelning av diff. maxima till vänster.

Alternativ lösning till: Vi använder Ewald konstruktion



Ewald sfären $r = k = \frac{2\pi}{\lambda}$

Reciproka gittret

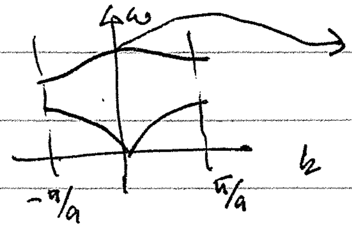
$\cos\theta_0 = \pi/2$ $\quad g_P = \frac{2\pi}{a}$

$\cos\theta_1 = \dfrac{\frac{2\pi}{a}}{k} = \dfrac{2\pi/a}{2\pi/\lambda} = \dfrac{\lambda}{a}$

$\cos\theta_2 = \dfrac{2 \cdot 2\pi/a}{k} = \dfrac{2 \cdot \frac{2\pi}{a}}{2\pi/\lambda} = \dfrac{2\lambda}{a}$

samma som tidigare

1c Dispersion relation för kristallen med 2 atomer i basen:



$$\hbar\omega_{max}^{optisk} = \hbar\omega_{max}^{o}(k=0) = \hbar\omega_{max}$$

Kolla kittel

$$\hbar\omega_{max}^{o}(k=0) = \hbar\sqrt{\frac{2C(M_1+M_2)}{M_1\cdot M_2}}$$

$$\Rightarrow \quad C = \frac{(\hbar\omega_{max})^2}{\hbar^2}\ \frac{M_1\cdot M_2}{2(M_1+M_2)} = \underline{\underline{1{,}5\ eV\text{Å}^{-2}}}$$

1d Optisk fonon med $\hbar\omega_{max}$ har $k=0$ i inelastisk neutron spridnings exp. gäller

energi bevaringen $\quad \frac{p_i^2}{2m} - \frac{p_f^2}{2m} = \hbar\omega_{max} \quad$ där $m \equiv$ neutron massa

rörelsemängd bev. $\quad p_i - p_f = (G+k)\hbar = \hbar\frac{2\pi l}{a} + 0 \quad l = 0,1,2$

i.e

$$\frac{p_i^2}{2m} - \frac{p_f^2}{2m} = \hbar\omega_f$$

$$p_i - p_f = \frac{l\cdot h}{2a} \qquad l = 1,2,3\ldots \quad h = \text{Planck konstant.}$$

Vi har system med 2 ekv. där vi söker p_i

Lösningen är

$$p_i = \frac{lh}{2a} + \frac{\hbar\omega_{max}\cdot m\cdot a}{lh}$$

Vi söker minimum för $p_i(l)$

$$\frac{dp_i}{dl} = 0 = \frac{h}{2a} - \frac{\hbar\omega_{max}\, m a}{l^2 h} = 0 \Rightarrow l^2 = \frac{\hbar\omega_{max}\, m\cdot 2a^2}{h^2}$$

Om vi använder $\hbar\omega_{max} = 30\,meV = 30\cdot 10^{-3}\cdot 1.6\cdot 10^{-19}\,J$

$$m = 1.6\cdot 10^{-27}\,kg$$

$$a = 5.64\cdot 10^{-10}\,m$$

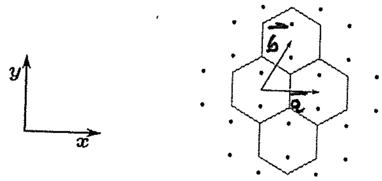
$$h = 6.6\cdot 10^{-34}\,J$$

$$\Rightarrow \quad n = 3.3 \Rightarrow n = 3$$

För $n=3 \Rightarrow E_i = \frac{p_i^2}{2m} = \underline{\underline{30.51\ meV}}$

2a Kristall = bas + gitter

gitter = trigonal Bravais
basen ≡ 2 atomer



2b $\vec{a} = d\sqrt{3}\,(1,0)$ $\quad$ $\vec{b} = d\sqrt{3}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$

$\vec{r}_1 = \left(0, \frac{d}{2}\right)$

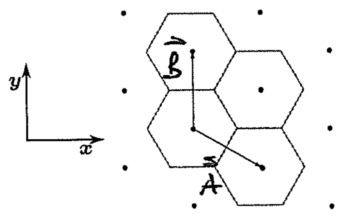
$\vec{r}_2 = (0, -d/2) = -\vec{r}_1$

2c Reciproka gitter vektorer $\vec{A}, \vec{B}$ fås från

$\vec{A}\cdot\vec{a} = 2\pi \qquad \vec{B}\cdot\vec{b} = 2\pi$

$\Rightarrow \quad \vec{A} = \frac{4\pi}{3d}\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right), \quad \vec{B} = \frac{4\pi}{3d}(0,1)$

$\vec{G}_{hk} = h\vec{A} + k\vec{B}$



2d $F_{hk} = NS = \sum_{j=1}^{2} f_j e^{i\vec{G}\cdot\vec{r}_j} = N\left(f e^{i\vec{G}\cdot\vec{r}_1} + f e^{i\vec{G}\cdot\vec{r}_2}\right)$

men $\vec{r}_1 = -\vec{r}_2$ $\qquad F_{hk} = Nf\left(e^{i\vec{G}\cdot\vec{r}_1} + e^{-i\vec{G}\cdot\vec{r}_1}\right) = Nf\cdot 2\cos\vec{G}\cdot\vec{r}_1$

$\vec{G} = h\vec{A} + k\vec{B} \qquad h,k \in \mathbb{Z}$

$\vec{r}_1 = \left(0, \frac{d}{2}\right)$

$\vec{G}\cdot\vec{r}_1 = \frac{\pi}{3}(2h-k)$

$I_{hk} = |F|^2 = N^2 f^2 \cdot 4\cos^2\left[\frac{\pi}{3}(2h-k)\right]$

2e $\quad k' = \vec{k} + \vec{G}$

$$e^{i\vec{k}'\cdot\vec{r}_{mn}} = e^{i(\vec{k}+\vec{G})\cdot\vec{r}_{mn}} = e^{i\vec{k}\cdot\vec{r}_{mn}} \cdot e^{i\vec{G}\cdot\vec{r}_{mn}} = e^{i\vec{k}\cdot\vec{r}_{mn}}$$

men $e^{i\vec{G}\cdot\vec{r}_{mn}} = 1$

$\Rightarrow e^{i\vec{k}'\cdot\vec{r}_{mn}}$ och $e^{i\vec{k}\cdot\vec{r}_{mn}}$ representerar samma vågrörelse