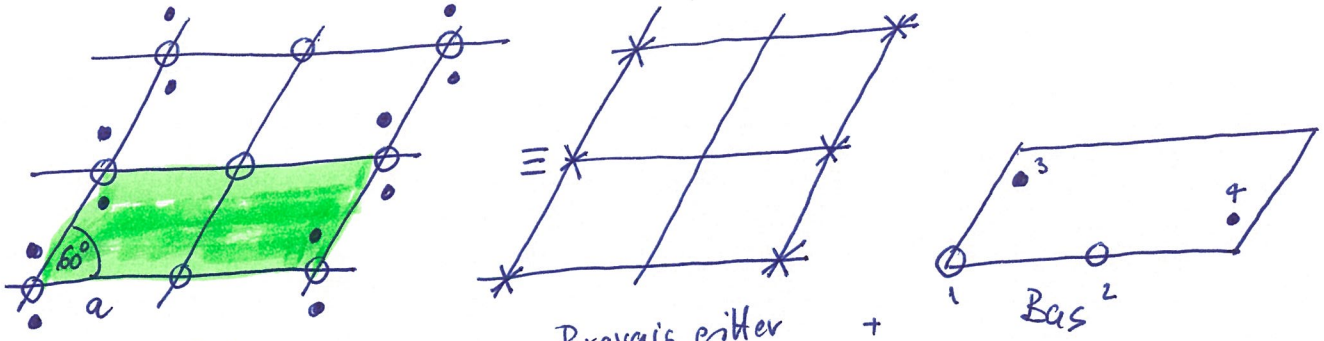
FTF.011 – Duggan 2012 02 09 – Lösningar

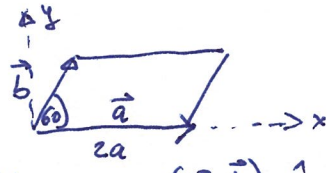
1a) Kristall ≡ gitter + bas



Kristall ≡ Bravais gitter + Bas

Bas ⇒ 4 atomer; 2st A-atomer + 2st B-atomer

1b) Primitiva gittertranslationsvektorer + basvektorer



$V_{cellen} = (\vec{a}\times\vec{b})\cdot\hat{z} = a^2\sqrt{3}$

$\vec{a} = 2a\hat{x}$

$\vec{b} = a\left(\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}\right)$

$\vec{R}_{mn} = m\vec{a} + n\vec{b}$

$\vec{R}_1 = (0,0,0)$

$\vec{R}_2 = (a, 0, 0)$

$\vec{R}_3 = \left(\frac{1}{2}a, \frac{a\sqrt{3}}{2}, 0\right)$

$\vec{R}_4 = (2a, 0, 0)$

bas vektorer

1c) Kemisk formel

B atomer i cellen = 2

A atomer i cellen = 1 + 1 = 2

A_2B_2

1d) Primitiva translationsvektorer i recipoka rummet:

$$\vec{A} = \frac{2\pi}{a^2\sqrt{3}}(\vec{b}\times\hat{z}) = \frac{2\pi}{a^2\sqrt{3}}\left(\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}\right)\times\hat{z} = \frac{\pi}{a}\left(\hat{x} - \frac{1}{\sqrt{3}}\hat{y}\right)$$

$$\vec{B} = \frac{2\pi}{a^2\sqrt{3}}(\hat{z}\times\vec{a}) = \frac{2\pi}{a^2\sqrt{3}}(\hat{z}\times 2a\hat{x}) = \frac{4\pi}{a\sqrt{3}}\hat{y}$$

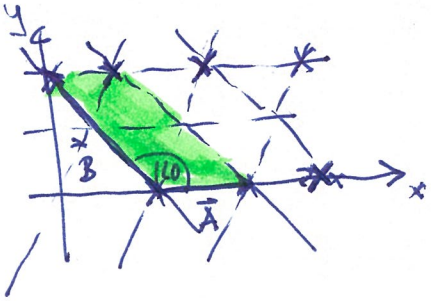
Test $\vec{a}\cdot\vec{A} = 2\pi$ ✓ $\vec{b}\times\vec{B} = 2\pi$ ✓ | $\vec{G}_{hk} = h\vec{A} + k\vec{B}$

Recipoka gittret:

$$|\vec{A}| = \frac{\pi}{a}\sqrt{1 + \tfrac{1}{3}} = \frac{\pi}{a}\sqrt{\tfrac{4}{3}} = \frac{2\pi}{a}\frac{1}{\sqrt{3}}$$

$$|\vec{B}| = 2\cdot\frac{2\pi}{a}\frac{1}{\sqrt{3}} = 2|\vec{A}|$$

$$\cos\sphericalangle(\vec{A},\vec{B}) = \frac{\vec{A}\cdot\vec{B}}{|\vec{A}|\cdot|\vec{B}|} = -\tfrac{1}{2} \Rightarrow \sphericalangle(\vec{A},\vec{B}) = 120°$$

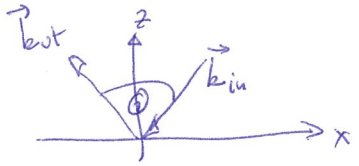


+ Stavar

(1c) Laue diffraktionsvillkor

(2D): $\vec{k}_{ut}^{\parallel} - \vec{k}_{in}^{\parallel} = \vec{G}_{hk}$ (1)

$k_{ut} = k_{in}$ (2)



$\vec{k}_{in} = (-k\cos 45, 0, -k\sin 45)$

$\vec{k}_{ut} = (k_{ut}^{x}, 0, k_{ut}^{z})$

från (1) $\Rightarrow$ $k_{ut}^{x} - k_{in}^{x} = G_{hk}^{x}$ (3)

$0 = G_{hk}^{y}$ (4)

men $\vec{G}_{hk} = h\frac{\pi}{a}\left(\hat{x} - \frac{1}{\sqrt{3}}\hat{y}\right) + k\frac{4\pi}{a\sqrt{3}}\hat{y}$

$\Rightarrow G_{hk}^{y} = 0 = -h\frac{\pi}{a}\frac{1}{\sqrt{3}} + k\frac{4\pi}{a\sqrt{3}} = 0 \Rightarrow k = \frac{h}{4}$

$\vec{G}_{hk}$ som ger diffraktion $= \vec{G}_{h\frac{h}{4}} = \frac{h\pi}{a}\hat{x}$ $\quad h = 4, 8, 12, \ldots$

Bragg vinklar θ?

$$\cos\theta = \frac{\vec{k}_{in}\cdot\vec{k}_{ut}}{|\vec{k}_{in}||\vec{k}_{ut}|} = \frac{\vec{k}_{in}\vec{k}_{ut}}{k^2} = \frac{k_{in}^{x}k_{ut}^{x} + k_{in}^{z}k_{ut}^{z}}{k^2}$$

Från (2) $\Rightarrow$ $k_{ut}^{x} = k_{in}^{x} + \frac{h\pi}{a} = -k\cos 45 + \frac{h\pi}{a}$

Från $k^2 = k_{ut}^{x2} + k_{ut}^{z2}$ $\Rightarrow$ $k_{ut}^{z} = \sqrt{k^2 - k_{ut}^{x2}} = \sqrt{k^2 - \left(-k\cos 45 + \frac{h\pi}{a}\right)^2}$

$$\cos\theta = \frac{(-k\cos 45)\left(-k\cos 45 + \frac{h\pi}{a}\right) + (-k\sin 45)\cdot\sqrt{k^2 - \left(-k\cos 45 + \frac{h\pi}{a}\right)^2}}{k^2}$$

$k = \frac{2\pi}{\lambda} = \frac{2\pi}{1.5} = 4.188\,\text{Å}^{-1}$

$\frac{\pi}{a} = \frac{\pi}{4.75} = 0.661\,\text{Å}^{-1}$

$h = 4 \Rightarrow \theta_1 = 130.60^\circ$

$h = 8 \Rightarrow \theta_2 = 169.1$ finns ej i reflektionen

$h = 12 \Rightarrow$ finns ej.

Intensiteten:

$$I_{hk} \propto |S|^2$$

$$S_{hk} = \sum_{j = \text{atomer i basen}} f_j e^{+i \vec{G}_{h,k/4} \cdot \vec{R}_j} \quad \rightarrow \text{basvektorer}$$

$$S_{41} = f_A \cdot e^{i \frac{4\pi}{a}\hat{x} \cdot (0,0,0)} + f_A e^{i \frac{4\pi}{a}\hat{x} \cdot (a,0,0)} + f_B e^{i \frac{4\pi}{a}\hat{x} \cdot \left(\frac{1}{2}a, \frac{a\sqrt{3}}{2}, 0\right)} +$$

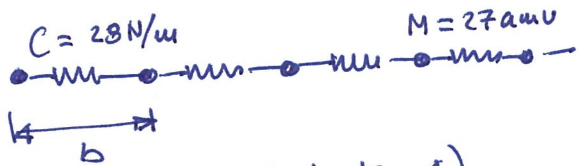
$$+ f_B e^{i \frac{4\pi \hat{x}}{a}(2a, 0, 0)}$$

$$S_{41} = f_A \cdot 1 + f_A e^{i4\pi} + f_B e^{i2\pi} + f_B e^{i8\pi} = 2f_A + 2f_B$$

$$I_{41} \propto |2f_A + 2f_B|^2$$

2a) [111] plan skovor $\Rightarrow$ $d_{111} = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{a}{\sqrt{3}} = \frac{4.05}{\sqrt{3}}$

$\Rightarrow b = \frac{4.05}{\sqrt{3}} = 2.34$ Å



Disp. relation (see Kittel Kap 4)

$$\omega^2 = \frac{4}{M} C \sin^2 \frac{kb}{2}$$

Ljudvågor: $k \to 0$ $\Rightarrow$ $\omega^2 \approx \frac{4C}{M} \frac{k^2 b^2}{4}$ $\Rightarrow$ $\omega = \sqrt{\frac{Cb^2}{M}} \cdot k$

$$v = \frac{d\omega}{dk} = \sqrt{\frac{Cb^2}{M}}$$

$C = 28$ N/m, $M = 27 \cdot 1.6 \cdot 10^{-27}$ kg, $b = 2.34 \cdot 10^{-10}$ m

$\Rightarrow$ $v = 5850$ m/s

2b) $\omega_{max}\ (kb = \pi) = \sqrt{\frac{4C}{M}} = 5 \cdot 10^{13} s^{-1}$

$\Rightarrow hf_{max} = \hbar\omega_{max} = 1.05 \cdot 10^{-34}\ Js \cdot 5 \cdot 10^{13} s^{-1} = 5.25 \cdot 10^{-21} J = \frac{5.25 \cdot 10^{-21} J}{1.6 \cdot 10^{-19} J/eV} = \approx 33 meV$

$k_B T$ vid $T = 300°K$ $\simeq$ 25 meV

$\hbar\omega_{max} = 33$ meV, $k_B T = 25$ meV $\Rightarrow$ ~~[struck out]~~ försumbar fermiskt exc.