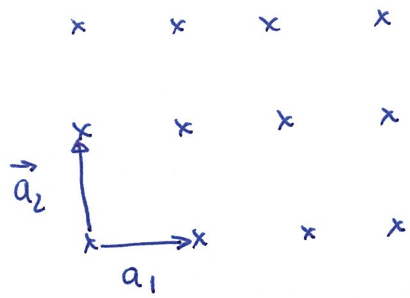
Lösningar till Duggan 100211

1) a)

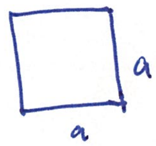
2D kvadratiskt Bravais gitter



$\vec{a}_1 = a\hat{i}$

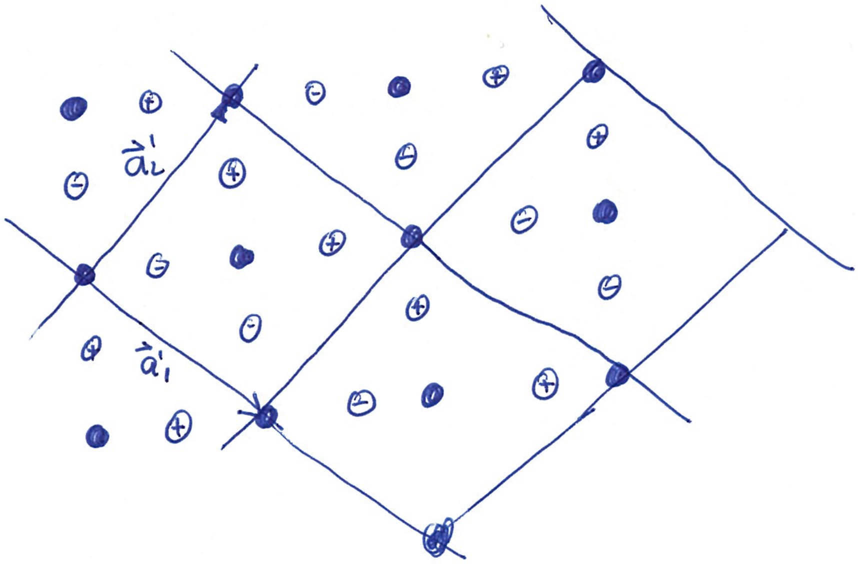
$\vec{a}_2 = a\hat{j}$

b) enhetscellen ⇒



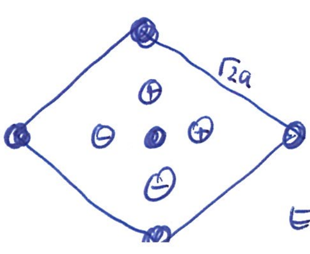
basen ⇒

c)



2D Bravais gitter:

Enhetscellen ⇒



Basen:

Enhetscellen innehåller 2st CuO_2 enheter

a) Rec. gitter till a)

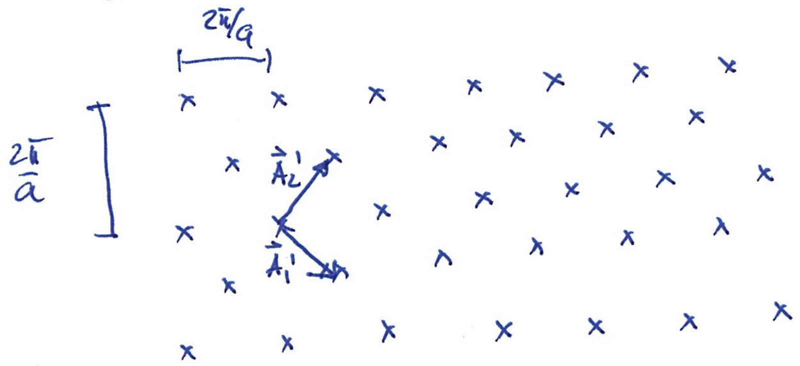
Bevis: $\vec{a}_i \cdot \vec{A}_j = \begin{cases} 2\pi\delta_{ij} & i=j \\ 0 & i \neq j \end{cases}$

$\vec{a}_i \in$ direkt gitter
$\vec{A}_j \in$ rec. gitter

$\vec{a}_1 = a\hat{i}$, $\vec{a}_2 = a\hat{j}$ $\Rightarrow$ $\vec{A}_1 = \frac{2\pi}{a}\hat{i}$, $\vec{A}_2 = \frac{2\pi}{a}\hat{j}$

Rec. gitter till b)

$$\left.\begin{aligned} \vec{a}_1' &= a(\hat{i}-\hat{j}) \\ \vec{a}_2' &= a(\hat{i}+\hat{j}) \end{aligned}\right\} \Rightarrow \begin{aligned} \vec{A}_1' &= \frac{2\pi}{a}(\hat{i}-\hat{j}) \\ \vec{A}_2' &= \frac{2\pi}{a}\hat{j}(\hat{i}+\hat{j}) \end{aligned}$$



2)

a) Kubiskt gitter, gitterparameter a, 2 atomer i basen

enhetscellen har volymen $V_c = a^3$ $\Rightarrow$ inom volymen V finns $N = \frac{V}{V_c}$ enhetsceller

$$I \propto |N|^2 \cdot |GS|^2 \cdot |S|^2$$

$$GS = 1 \quad \text{om} \quad \vec{\Delta k} = \vec{G}$$

$$S = 2f \quad \text{eller} \quad 0$$

$$\Rightarrow \quad I \propto 4N^2 f^2 \quad \text{där} \quad N = \frac{V}{a^3}$$

b) primitivt romboedriskt gitter med volymen $\underline{\underline{\frac{1}{2}a^3}}$

$\Rightarrow$ i volymen V finns $\frac{V}{\frac{1}{2}a^3} = 2\frac{V}{a^3} = 2N$ ~~celler~~ primitiva enhetsceller

$$GS = 1, \quad S = f \quad \text{(en atom i basen)}$$

$$I \propto |N'|^2 |GS|^2 |S|^2 = (2N)^2 \cdot 1^2 \cdot f^2 = 4N^2 f^2$$

i. e. samma som i a)

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3) a) Bandgapet vid BZ kanten är

$$\Delta\omega = \sqrt{\frac{2C}{M_{Cl}}} - \sqrt{\frac{2C}{M_{Pt}}} \Rightarrow C = \frac{1}{2}\frac{\Delta\omega^2}{\left(\sqrt{\frac{1}{M_{Cl}}} - \sqrt{\frac{1}{M_{Pt}}}\right)^2}$$

$$C = 7.26 \text{ kg/s}^2 = 7.26 \frac{\text{kg m}^2}{\text{m}^2 \text{s}^2} = 7.26 \frac{\text{J}}{\text{m}^2} = 0.453 \frac{\text{eV}}{\text{Å}^2}$$

b) $$v_{ak} = \frac{\omega_{ak}(k \to 0)}{k} = a\sqrt{\frac{C}{(M_{Pt} + M_{Cl})}}$$

$$v_{ak} = \underline{\underline{832 \text{ m/s}}}$$

4 Rörelse ekv.:

$$M\ddot{u}_s = \underbrace{C_1(u_{s+1}+u_{s-1}-2u_s)}_{\text{harmonisk kraft mellan ng}} + \underbrace{C_2(u_{s+2}+u_{s-2}-2u_s)}_{\text{harm. kraft mellan n.n.g.}} + \underbrace{C_3(u_{s+3}+u_{s-3}-2u_s)}_{\text{harm. kraft mellan n.n.n.g.}}$$

Ansatz $u = u_0 e^{i(ksa-\omega t)}$ matas in i rörelse ekv. $\Rightarrow$

$$-M\omega^2 = C_1(e^{ika}+e^{-ika}-2) + C_2(e^{i2ka}+e^{-i2ka}-2) + C_3(e^{i3ka}+e^{-i3ka}-2)$$

$$\omega^2 = \frac{4}{M}\left(C_1 \sin^2\frac{ka}{2} + C_2 \sin^2\frac{2ka}{2} + C_3 \sin^2\frac{3ka}{2}\right)$$

Ljudvågor: $v_{ak} = \dfrac{\omega(k\to 0)}{k}$

om $k \to 0 \Rightarrow ka \ll 1 \Rightarrow \sin ka \approx ka$

$$\Rightarrow \omega^2 \approx \frac{4}{M}\left[C_1\left(\frac{ka}{2}\right)^2 + C_2\left(\frac{2ka}{2}\right)^2 + C_3\left(\frac{3ka}{2}\right)^2\right]$$

$$\omega^2 = \frac{(ka)^2}{M}\left(C_1 + 4C_2 + 9C_3\right)$$

$$v_{ak} = \frac{a}{\sqrt{M}}\sqrt{C_1+4C_2+9C_3} = \underline{6{,}6\cdot 10^3\ m/s}$$

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5) i jämvikten gäller:

U_{Total} = minimum då $r = \frac{a}{2}$ dvs avståndet mellan Na^+ och Cl^- joner i NaCl kristallen

$$\Rightarrow \left.\frac{dU_{Tot}}{dr}\right|_{r=a/2} = 0$$

$$\Rightarrow \left.\begin{matrix}\dfrac{1}{4\pi\varepsilon_0}\dfrac{\alpha e^2}{r^2} - \dfrac{12C}{r^{13}} = 0 \\ r = a/2\end{matrix}\right\} \Rightarrow C = \frac{1}{12}\frac{1}{4\pi\varepsilon_0}\alpha e^2\left(\frac{a}{2}\right)^{11}$$

$$C = 2{,}95\cdot 10^{-134}\ Jm^{12} = \underline{1.85\cdot 10^{5}\ eV\text{Å}^{12}}$$