LECTURE #13

Note Title 10/15/2008

HEXAGONAL LATTICE 2D

HCP LATTICE

RECIPROCAL LATTICE $e^{i\vec{K}\cdot\vec{r}}$ SAME SYMMETRY OF THE LATTICE

(*) $e^{i\vec{K}\cdot\vec{R}_i} = 1 \quad \forall \vec{R}_i$ ($\vec{R}_i$ POSITION ATOMS IN DIRECT LATTICE)

MANY $\vec{K}_J$ THAT SATISFY (*)

$\{\vec{K}_J\}$ IS A LATTICE $\rightarrow$ RECIPROCAL LATTICE

$\{\vec{R}_i\}$ BRAVAIS $\longrightarrow$ $\{\vec{K}_J\}$ ALSO BRAVAIS

$$\vec{R}_i = m_1 \vec{a}_1 + m_2 \vec{a}_2 + m_3 \vec{a}_3$$

$$\vec{K}_j = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3$$

GIVEN $\vec{a}_1, \vec{a}_2, \vec{a}_3$ HOW DO YOU FIND $\vec{b}_1, \vec{b}_2, \vec{b}_3$?

FOCUS ON POINT $\vec{b}_1$

$$e^{i \vec{R}_i \cdot \vec{b}_1} = 1 \Rightarrow \vec{R}_i \cdot \vec{b}_1 = 2\pi \text{ integer} \quad \forall \vec{R}_i$$

$$(m_1 \vec{a}_1 + m_2 \vec{a}_2 + m_3 \vec{a}_3) \cdot \vec{b}_1 = 2\pi \text{ integer}$$

$$\vec{a}_1 \cdot \vec{b}_1 = 2\pi, \quad \vec{a}_2 \cdot \vec{b}_1 = 0, \quad \vec{a}_3 \cdot \vec{b}_1 = 0$$

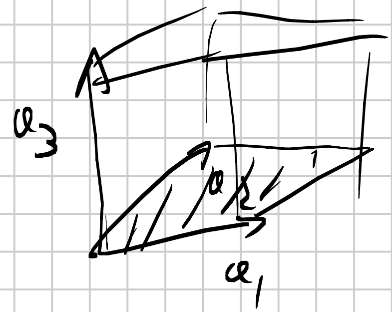
$$\Rightarrow \vec{R}_i \cdot \vec{b}_1 = 2\pi m_1$$

$$\begin{cases} \vec{b}_1 \perp \vec{a}_2 \text{ AND } \vec{a}_3 \Rightarrow \vec{b}_1 = c\,(\vec{a}_2 \times \vec{a}_3) \\ \vec{b}_1 \cdot \vec{a}_1 = 2\pi \Rightarrow c\,(\vec{a}_2 \times \vec{a}_3) \cdot \vec{a}_1 = 2\pi \Rightarrow c = \dfrac{2\pi}{|(\vec{a}_2 \times \vec{a}_3) \cdot \vec{a}_1|} \end{cases}$$

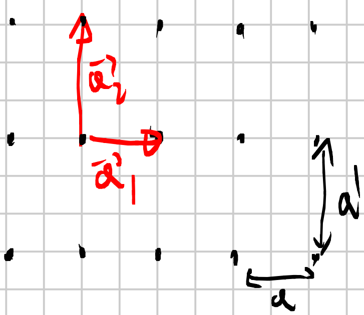
$$\vec{b}_1 = \frac{2\pi}{\left|(\vec{a}_2 \times \vec{a}_3)\cdot \vec{a}_1\right|}\left(\vec{a}_2 \times \vec{a}_3\right)$$

$$\vec{b}_i = \frac{2\pi}{\left|(\vec{a}_2 \times \vec{a}_3)\cdot \vec{a}_1\right|}\left(\vec{a}_j \times \vec{a}_k\right) \qquad i, j, k \in \{1, 2, 3\}$$

$$\left|(a_1 \times a_2)\cdot a_3\right| = V_{\text{UNIT CELL}}$$



FOR A 2D LATTICE TAKE $\vec{a}_3 = c\,\hat{z}$

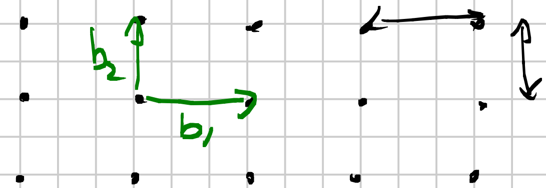


DIRECT

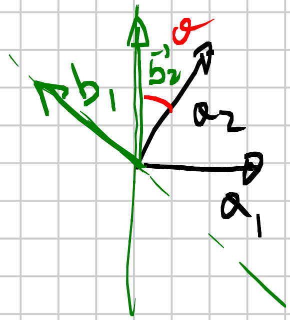
$b_1 \cdot a_1 = 2\pi$

$b_2 \cdot a_2 = 2\pi$

$b = \frac{2\pi}{a}$



$b' = \frac{2\pi}{a'}$



$$\vec{b}_2 \cdot \vec{a}_2 = 2\pi$$

$$|b_2|\,|a_2| \cos\theta = 2\pi$$

$\boxed{\text{IN 3D}}$

RECIPROCAL LATTICE

SIMPLE CUBIC a $\Rightarrow$ SIMPLE CUBIC $\frac{2\pi}{a}$

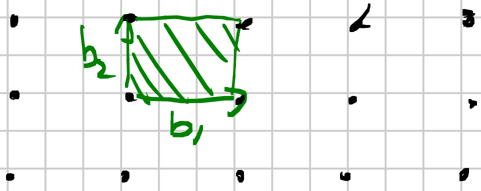
FCC SIDE a $\Rightarrow$ BCC SIDE $\frac{4\pi}{a}$

BCC SIDE a $\Rightarrow$ FCC SIDE $\frac{4\pi}{a}$

HEX SIDE TRIANGLES a $\Rightarrow$ HEX SIDE $\frac{2\pi}{a}\sqrt{\frac{4}{3}}$

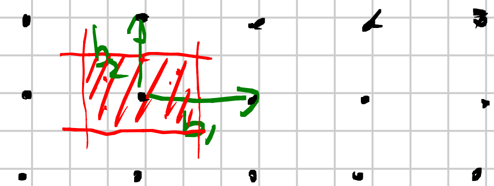
1° BRILLOUIN ZONE

CONVENTIONAL UNIT CELL FOR RECIPROCAL LATTICE



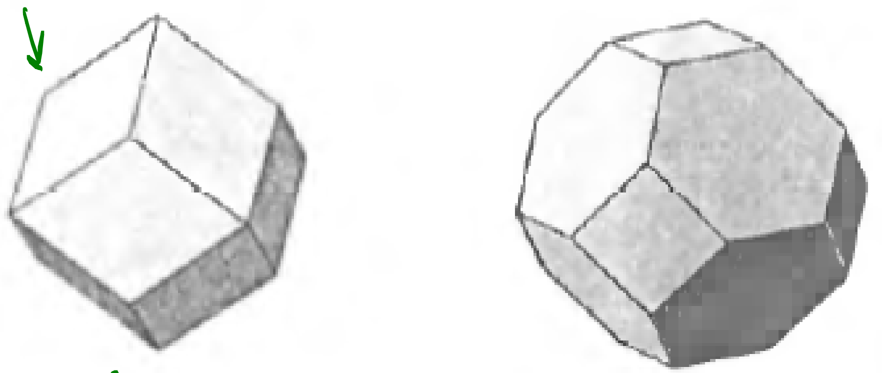
WIGNER-SEITZ CELL FOR THE RECIPROCAL LATTICE

= 1ST BRILLOUIN ZONE



1° BZ FOR BCC

1° BZ FOR FCC



DODECAHEDRON

(a) (b)

DIRECT SPACE

WS CELL FOR

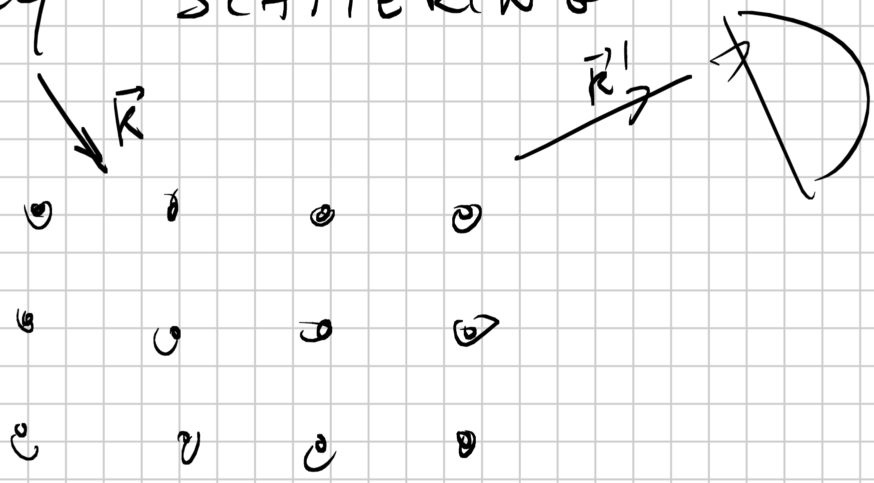
BCC → OCTAHEDRON

FCC → DODECAHEDRON

RECIPROCAL LATTICE

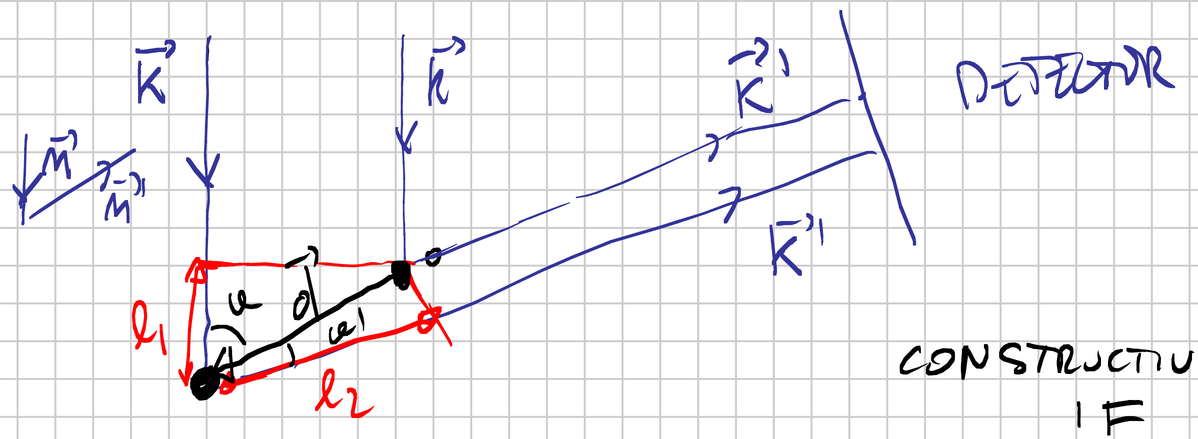
FCC ⇄ BCC

X-RAY SCATTERING



LOOK FOR CONSTRUCTIVE INTERFERENCE OF LIGHT SCATTERED FROM ATOMS

2 ATOMS



CONSTRUCTIVE INTERFERENCE IF

OPTICAL PATH DIFFERENCE $= \delta = m\lambda = l_1 + l_2$

$$l_1 = d\cos\theta = \vec{d}\cdot\vec{m}$$

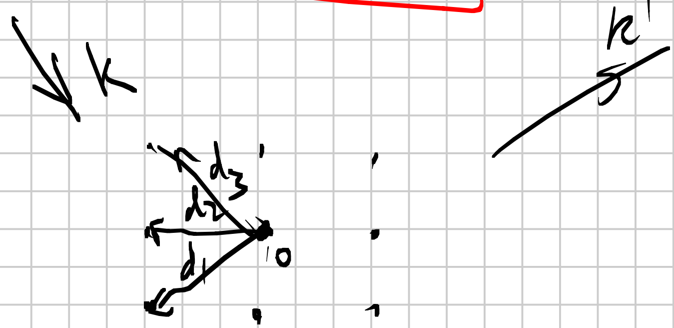
$$l_2 = d\cos\theta' = -\vec{d}\cdot\vec{m}'$$

$$\delta = \vec{d}\cdot(\vec{n}-\vec{n}') = m\lambda \qquad e^{i\vec{k}\cdot\vec{r}} \qquad e^{i\vec{n}\, r\frac{2\pi}{\lambda}}$$

$|\vec{k}| = \frac{2\pi}{\lambda}$ ELASTIC SCATTERING $|\vec{k}'| = \frac{2\pi}{\lambda}$

$$\boxed{\vec{d}\cdot(\vec{k}-\vec{k}') = 2\pi m}$$

CONDITION FOR 2 ATOMS



$\vec{d}_i\cdot(\vec{k}-\vec{k}') = 2\pi m \quad \forall\, \vec{d}_i$ IN THE SYSTEM

CRYSTAL $\{\vec{R}_i\}$ POSITION ALL ATOMS CRYSTAL

$$\vec{R}_i \cdot (\vec{k} - \vec{k}') = 2\pi m \quad \forall R_i \Rightarrow$$ CONSTRUCTIVE INTERFERENCE FROM ALL ATOMS IN THE CRYSTAL

$$\vec{R}_i \cdot \vec{K} = 2\pi m$$

$$\boxed{\vec{k} - \vec{k}' = \vec{K}}$$