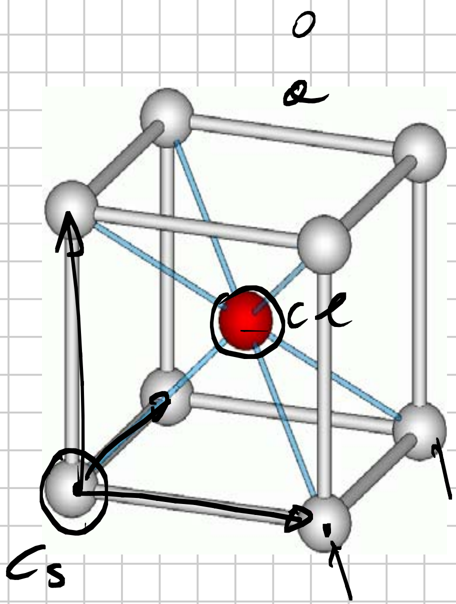
Lecture # 11

Note Title 10/15/2007



Not a BCC!

Simple cubic

$\vec{a}_1 = a(100)$

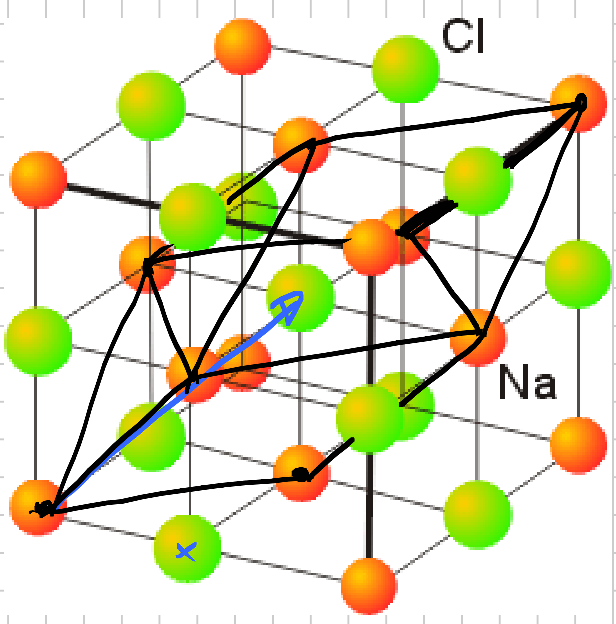
$\vec{a}_2 = a(010)$

$\vec{a}_3 = a(001)$

$$\begin{cases} \vec{b}_{Cs} = (0,0,0) \\ \vec{b}_{Cl} = \frac{a}{2}(111) \end{cases}$$

Volume of unit cell $= a^3$

Density: $\frac{2 \text{ atoms}}{a^3}$



Not a SC

Look at Na → FCC

$a_1 = \frac{a}{2}(110)$

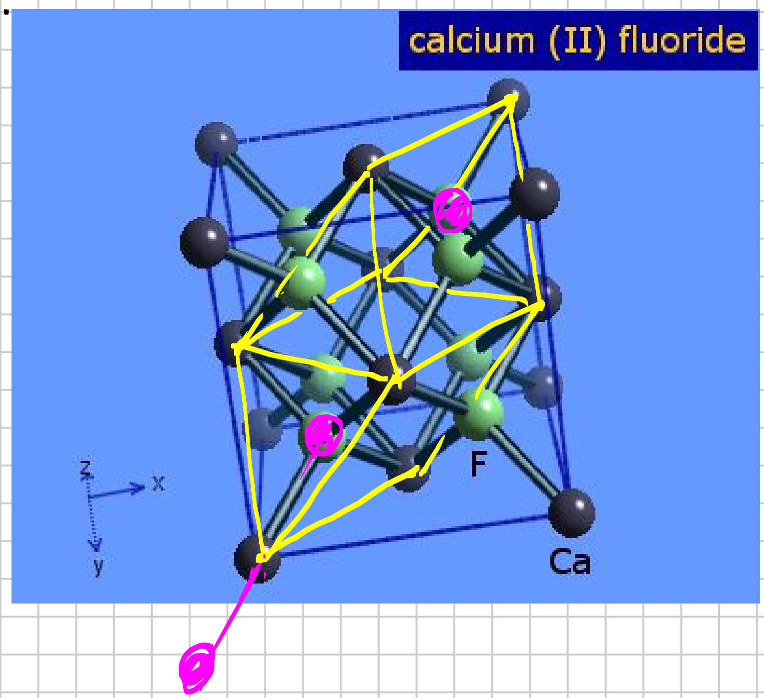
$a_2 = \frac{a}{2}(011)$

$a_3 = \frac{a}{2}(101)$

volume $= \frac{a^3}{4}$

$$\begin{cases} \vec{b}_{Na} = (0,0,0) \rightarrow \text{FCC} \\ \vec{b}_{Cl} = \frac{a}{2}(111) \rightarrow \text{FCC} \end{cases}$$

$n = \frac{2}{a^3/4} = \frac{8}{a^3}$



① Ca make an FCC

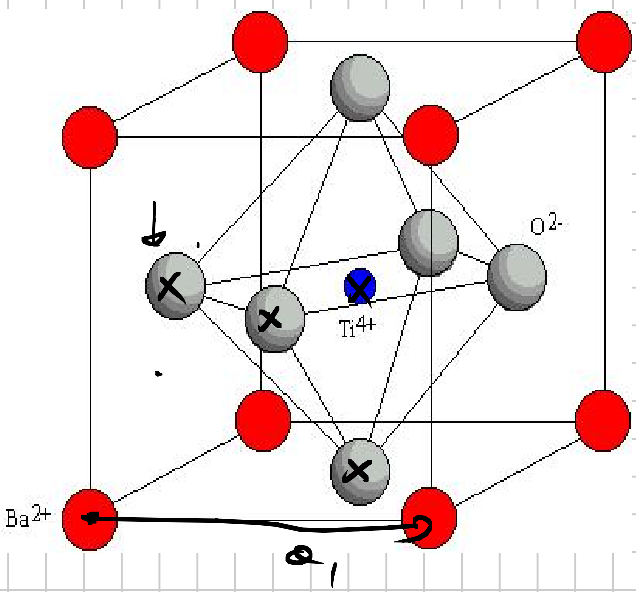
$a_1 = \frac{a}{2}(1\,1\,0)$
$a_2 = \frac{a}{2}(0\,1\,1)$
$a_3 = \frac{a}{2}(1\,0\,1)$

$\vec{b}_{Ca} = (0,0,0)$

$\vec{b}_F = \frac{a}{4}(1\,1\,1)$

$\vec{b}_F = 3\frac{a}{4}(1\,1\,1)$

$\frac{3 \text{ atoms}}{a^3/4}$



Simple Cubic

$b_{Ba} = (0\,0\,0)$

$b_o = \frac{a}{2}(1\,1\,0)$

$b_o = \frac{a}{2}(1\,0\,1)$

$b_o = \frac{a}{2}(0\,1\,1)$

$b_{Ti} = \frac{a}{2}(1\,1\,1)$

$\frac{5 \text{ Atoms}}{a^3}$

Hexagonal lattice

HCP crystal structure

RECIPROCAL LATTICE

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

Bravais Bravais

$$e^{i\vec{K}_J \cdot \vec{R}_i} = 1$$

$K_i \rightarrow$ wave with same symmetry of lattice

$$\vec{R}_i = \left(n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3\right)$$

$$\vec{K}_J = \left(m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3\right)$$

$\boxed{\vec{b}_1 \quad \vec{b}_2 \quad \vec{b}_3}$

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

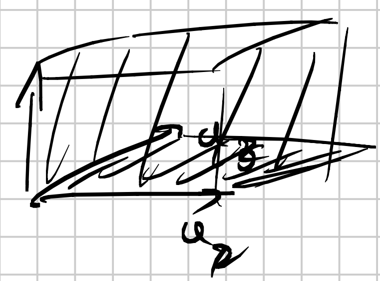
$$\left(n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3\right) \cdot \left(m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3\right) = 2\pi K$$

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

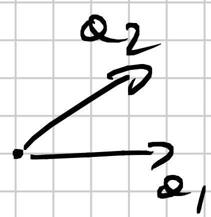
$$\vec{b}_1 = \frac{2\pi \left(\vec{a}_2 \times \vec{a}_3\right)}{\vec{a}_1 \cdot \left(\vec{a}_2 \times \vec{a}_3\right)}$$

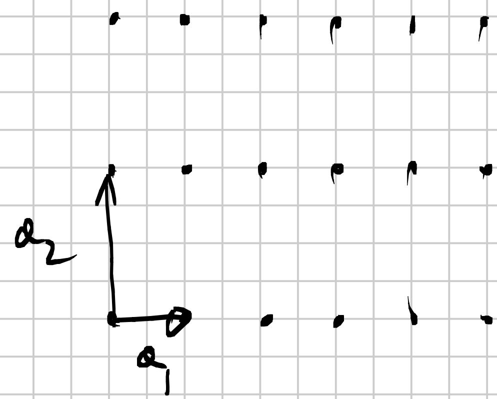
$$\vec{b}_i = \frac{2\pi \left(\vec{a}_j \times \vec{a}_k\right)}{\vec{a}_1 \cdot \left(\vec{a}_2 \times \vec{a}_3\right)} \qquad i\, j\, k \in \{1, 2, 3\}$$

$$\vec{a}_1 \cdot \left(\vec{a}_2 \times \vec{a}_3\right) = \text{volume unit cell}$$



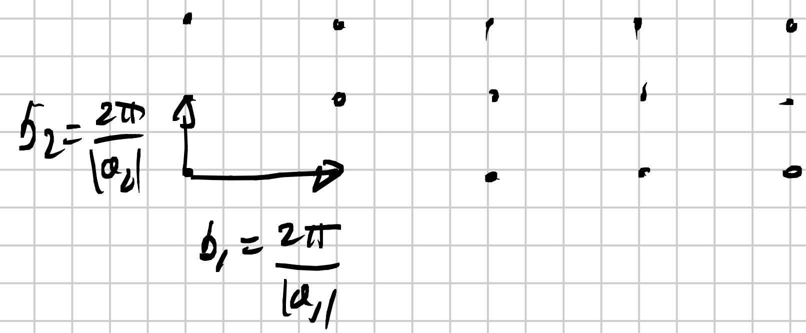
For a 2D lattice (add $\hat{z}$ as $\vec{a}_3$)





Direct

$b_1 \cdot a_1 = 2\pi \qquad b_2 \cdot a_2 = 2\pi$



IN 3D

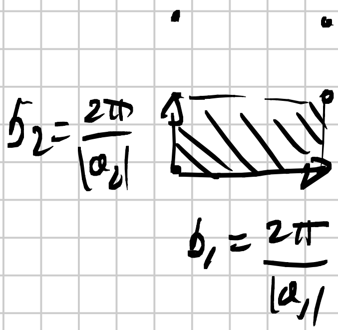
S Cubic $a \longrightarrow$ S Cubic $\frac{2\pi}{a}$

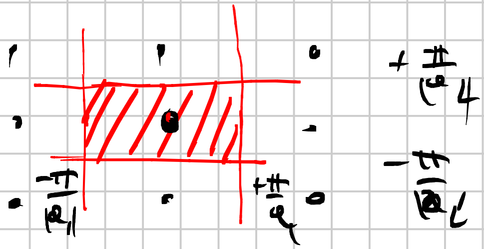
FCC $a \longrightarrow$ BCC $\frac{4\pi}{a}$

BCC $a \longrightarrow$ FCC $\frac{4\pi}{a}$

HEX $a \longrightarrow$ HEX $\frac{2\pi}{a}\sqrt{\frac{4}{3}}$

Unit Cell of Reciprocal Lattice





WIGNER-SEITZ UNIT CELL OF RECIPROCAL LATTICE

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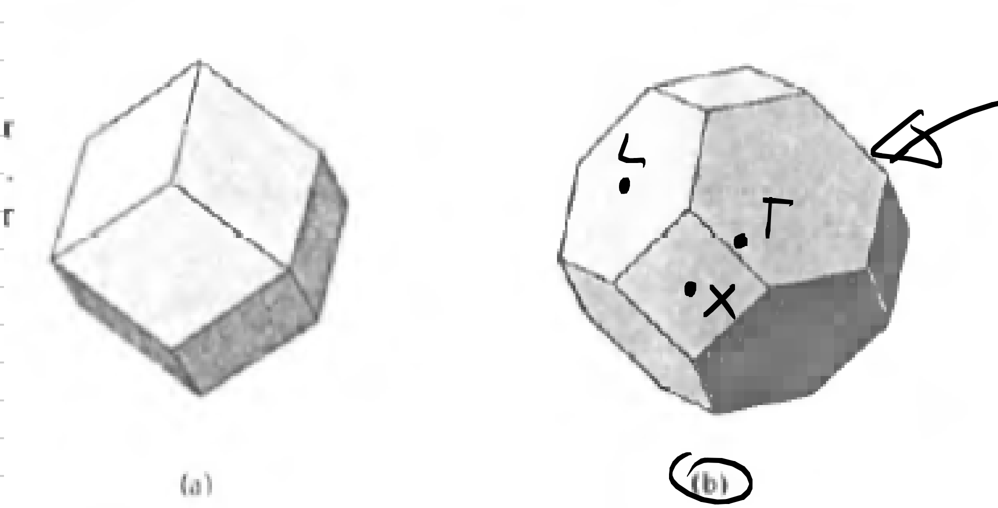
1° BRILLOUIN ZONE



(a) DODECAHEDRON

(b) OCTAHEDRON

DIRECT : FCC

⇓

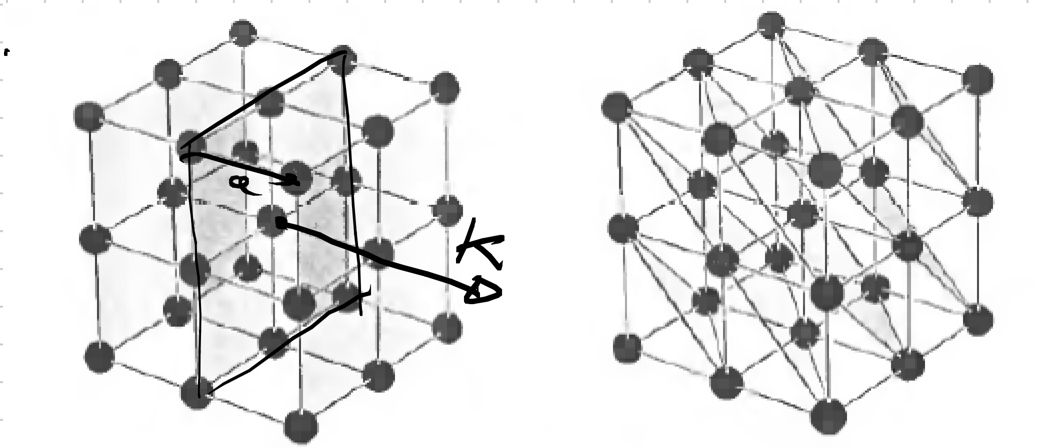
RECIPROCAL BCC

REC FCC

↓

DIRECT BCC

LINK BETWEEN $\vec{K}$ AND FAMILY OF PLANES IN A BRAVAIS LATTICE



(a) (b)

$\longrightarrow \vec{K}$ (111)

$\vec{K} \perp$ TO FAMILY OF PLANES

$$|\vec{K}| = \frac{2\pi}{d}$$

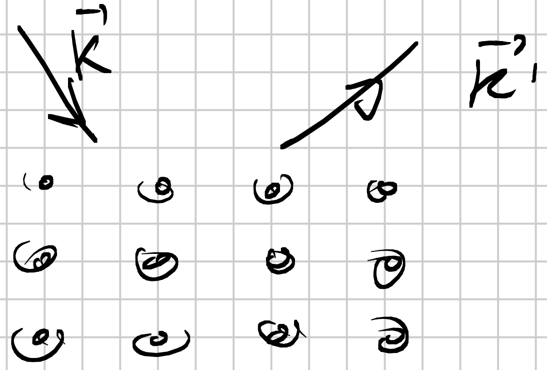
d distance between planes

Reciprocal lattice points

K:

important in Scattering

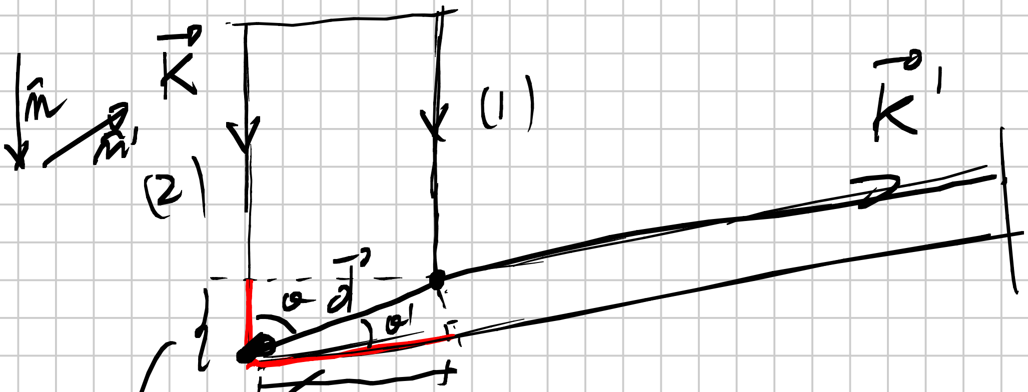
X-RAYS



Look first at 2 atoms

Difference in paths

$$\delta = m\lambda$$



$$d\cos\theta = \vec d\cdot\hat n$$

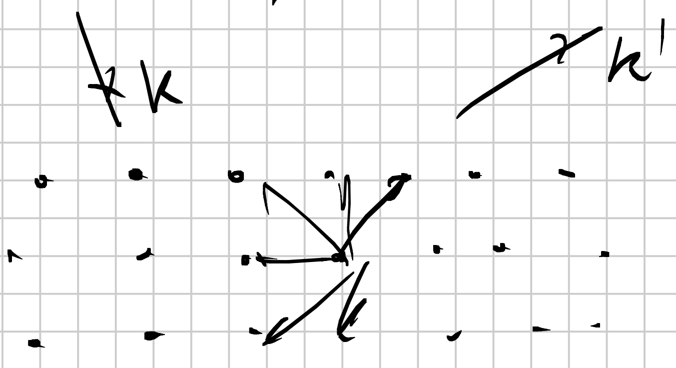
$$d\cos\theta' = -\vec d\cdot\hat n'$$

$$\delta = \vec d\cdot(\hat n - \hat n') = m\lambda$$

k

$$\frac{2\pi}{\lambda}$$

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



$$\vec{R}_i \cdot (\vec{k}-\vec{k}') = 2\pi m \quad \forall R_i$$

$$\Downarrow$$

$$(\vec{k}-\vec{k}') = K$$ IS A VECTOR OF RECIPROCAL LATTICE

Chap 4 Chap 7
Chap 5

→ Ashcroft Mermin