LECTURE # 12

Note Title 10/13/2008

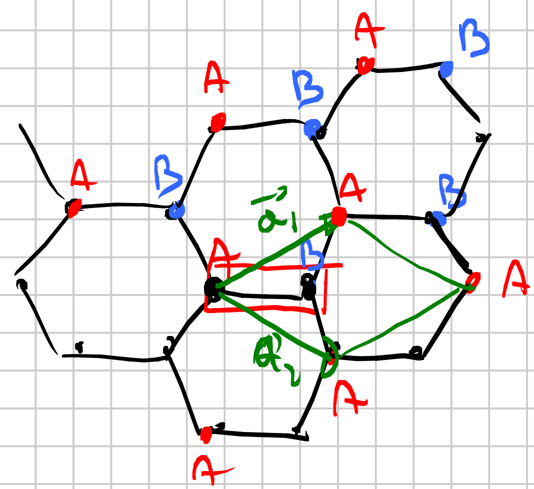
CRYSTAL STRUCTURES

① BRAVAIS LATTICE – SAME "VIEW" – $\vec{a}_1, \vec{a}_2, \vec{a}_3$ PRIMITIVE VECTORS

ONE ATOM PER UNIT CELL

② LATTICE WITH A BASIS

MORE THAN 1 ATOM PER UNIT CELL



HONEYCOMB

SUBLATTICE A +

SUBLATTICE B

2 ATOMS

CUBIC
FCC
BCC

} BRAVAIS

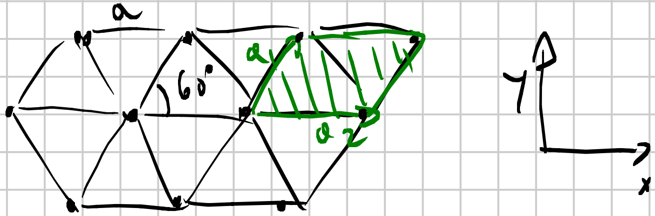
DIAMOND / ZINCBLENDE

FCC

$\vec{b}_A = 0$

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

a SIDE CUBE



2D HEXAGONAL LATTICE

$\vec{a}_1 = a(1,0)$

$\vec{a}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$

3D HEXAGONAL LATTICE

BRAVAIS

$\vec{a}_1 = a(1,0,0)$

$\vec{a}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right)$

$\vec{a}_3 = c(0,0,1)$

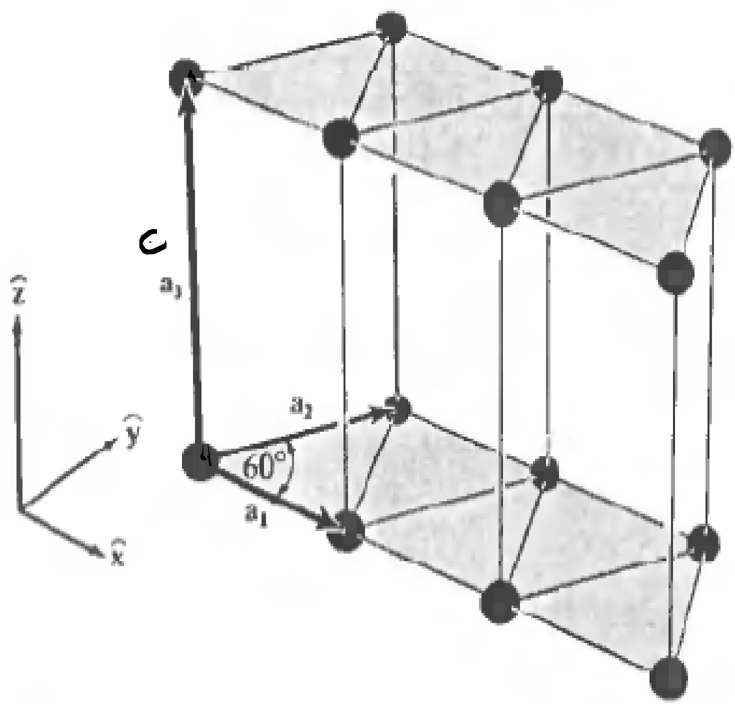
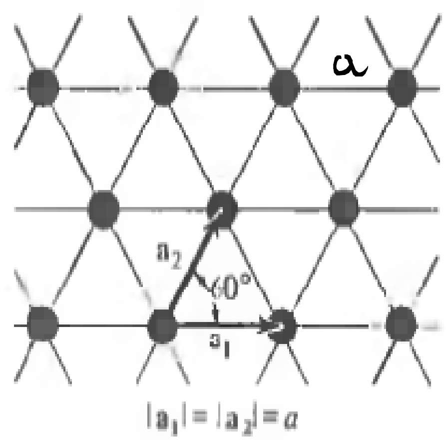
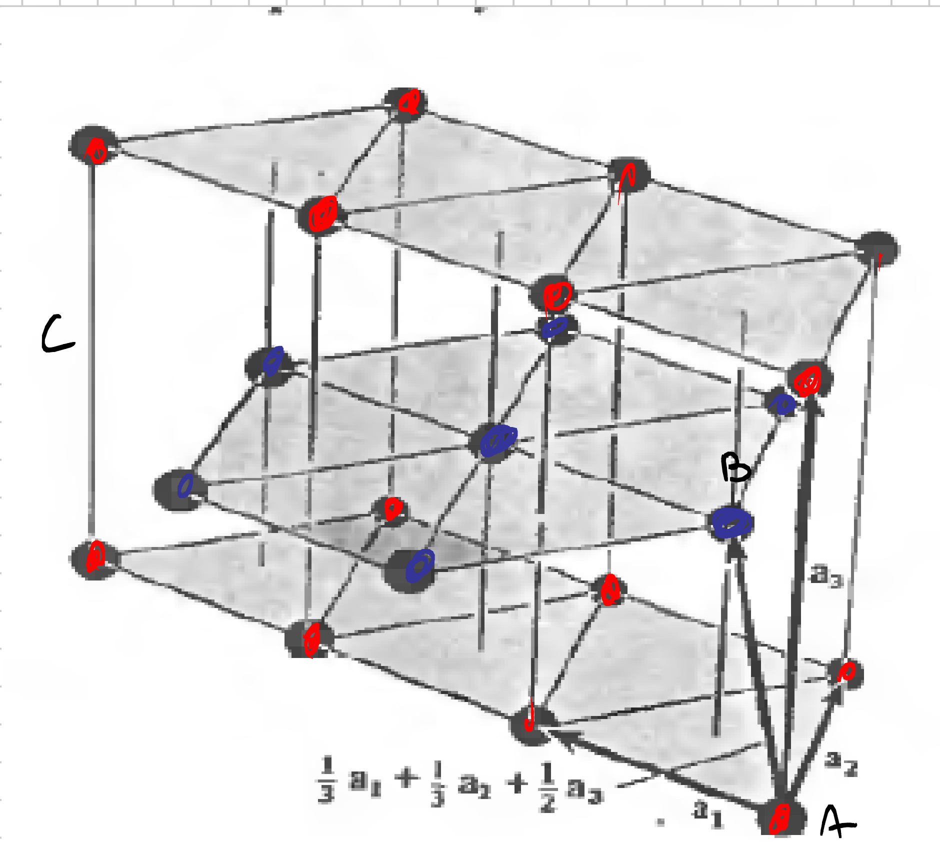


Figure 4.19



HEXAGONAL - CLOSED - PACKED HCP

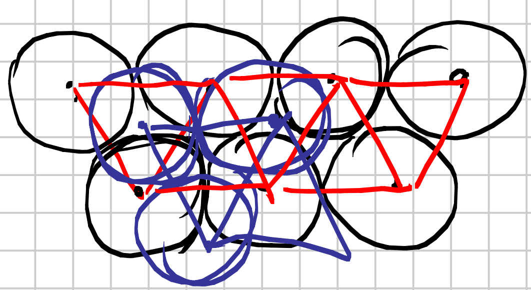


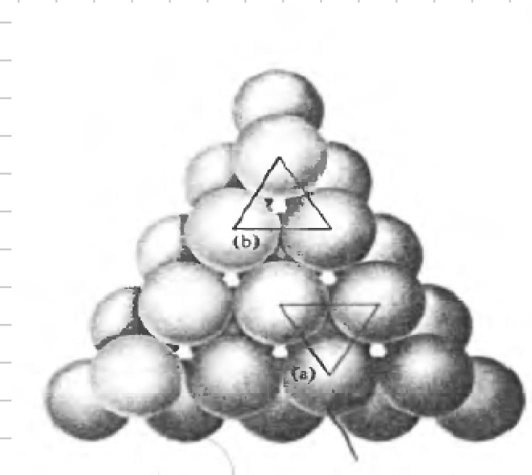
WURZITE

CdS

$$\left[\begin{array}{l} \vec{b}_A = 0 \\ \vec{b}_B = \dfrac{\vec{a}_3}{2} + \dfrac{\vec{a}_2}{3} + \dfrac{\vec{a}_1}{3} \end{array}\right]$$

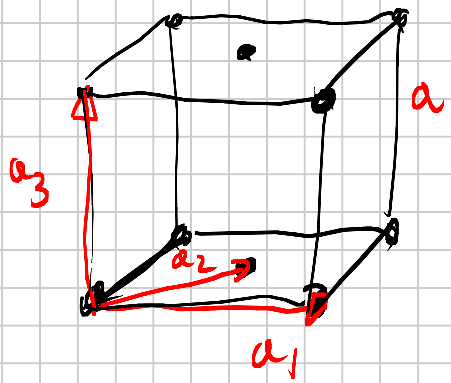
STACK OF CANNON - BALLS





WHAT IS c ?

$$\frac{c}{a} = \sqrt{\frac{8}{3}}$$



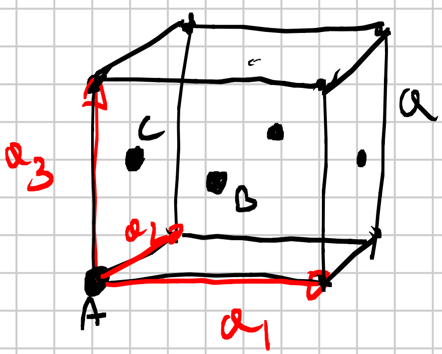
BASE CENTERED CUBIC

YES BRAVAIS

$\vec{a}_1 = a(1\ 0\ 0)$ $\qquad V = \frac{a^3}{2}$

$\vec{a}_2 = a(\frac{1}{2}\ \frac{1}{2}\ 0)$

$\vec{a}_3 = a(0\ 0\ 1)$ $\qquad n = \frac{2}{a^3}$



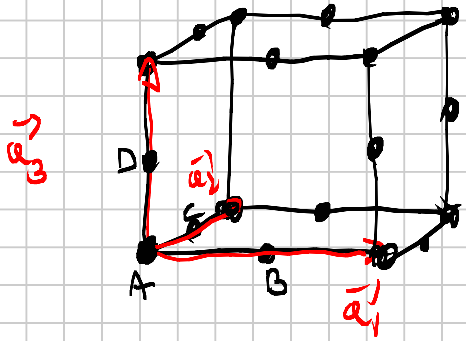
NOT BRAVAIS

3 ATOMS / UNIT CELL

$\vec{b}_A = 0$

$\vec{b}_B = \frac{a}{2}(1\ 0\ 1)$ $\qquad n = \frac{3}{a^3}$

$\vec{b}_C = \frac{a}{2}(0\ 1\ 1)$



NOT BRAVAIS

4 ATOMS IN THE UNIT CELL

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

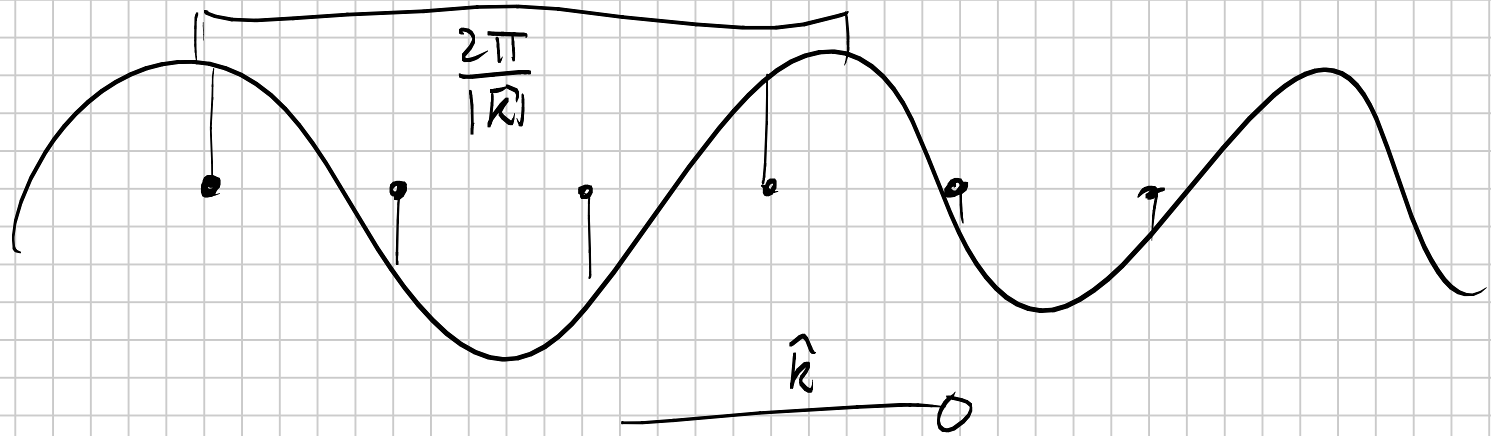
$b_A = 0$

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

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

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

Chapt. 5



$e^{i\vec{k}\cdot\vec{r}}$

$\vec{k}$

IN GENERAL NO MATCHING BETWEEN λ AND LATTICE SYMMETRY

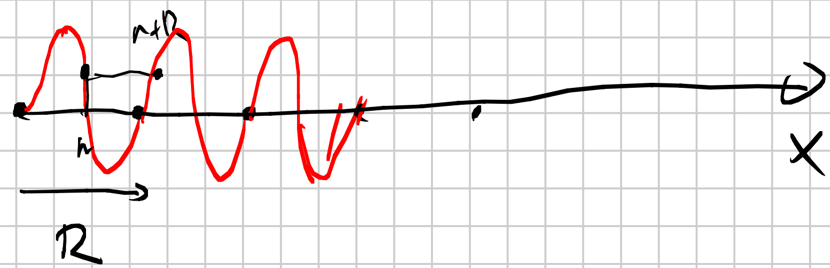
SPECIAL VALUES OF $\vec{K}$ TO MATCH THE

LATTICE SYMMETRY

$\{\vec{R}_i\}$ SET OF POINTS DEFINING THE BRAVAIS LATTICE

$$e^{i\vec{K}\cdot\vec{r}} = e^{i\vec{K}\cdot(\vec{r}+\vec{R}_i)} \quad \forall \vec{R}_i$$

$$e^{i\vec{K}\cdot\vec{R}_i} = 1 \quad \forall \vec{R}_i \text{ IN THE BRAVAIS LATTICE}$$



ALL $\vec{K}_J$ SUCH THAT

$\vec{K}_J \cdot \vec{R}_i = 2\pi m$ MAKE A LATTICE

$\{\vec{K}_J\}$ CALLED RECIPROCAL LATTICE OF $\{\vec{R}_i\}$

$\{R_i\}$ BRAVAIS LATTICE $\longrightarrow$ $\{\vec{K}_J\}$ ALSO A BRAVAIS LATTICE

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

$m_i \in \mathbb{Z}$

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

$\vec{b}_1, \vec{b}_2, \vec{b}_3$

PRIMITIVE VECTORS OF THE RECIPROCAL LATTICE

$$\vec{R}_i \cdot \vec{K}_J = 2\pi N \qquad \forall \vec{R}_i$$

$N \in \mathbb{Z}$

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

LOOK AT $\vec{b}_1$ CONSIDER $m_1 = 1$ $m_2 = 0$ $m_3 = 0$

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

① $\vec{b}_1 \perp \vec{a}_2$ AND $\vec{a}_3 \Rightarrow \vec{b}_1 = c\left(\vec{a}_2 \times \vec{a}_3\right)$

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

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

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

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

$$c = \frac{2\pi}{\text{VOLUME UNIT CELL}}$$

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

$i, j, k \in 1, 2, 3$