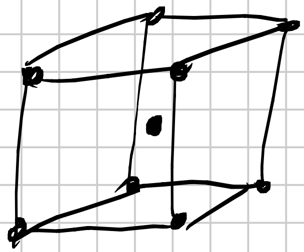
LECTURE #10

Note Title 10/10/2007

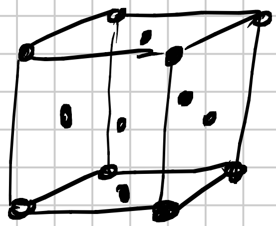
BRAVAIS LATTICE

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

$\left.\begin{array}{l}\vec{a}_1\\ \vec{a}_2\\ \vec{a}_3\end{array}\right\}$ Primitive vectors

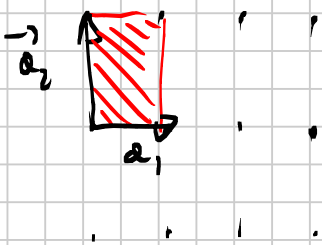


BCC

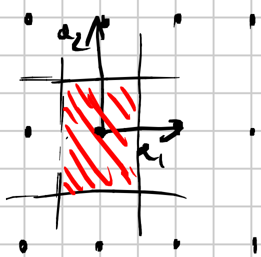


FCC

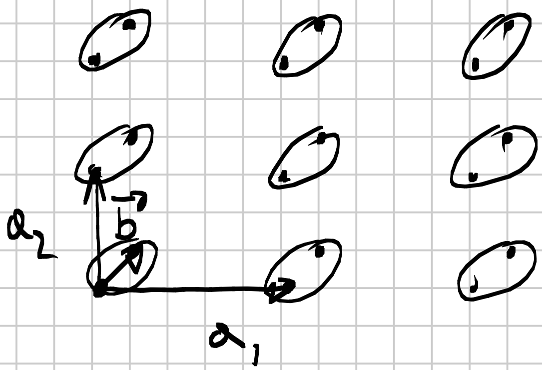
Primitive unit cell



Wigner-Seitz cell



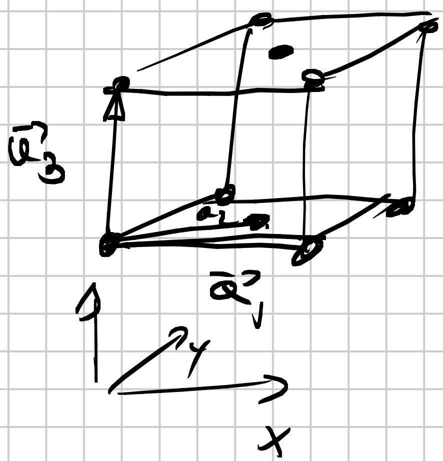
Many crystal structures are NOT Bravais lattices but can be described as "Bravais lattices with basis"



$\vec{b}$ BASIS

2 ATOMS IN THE BASIS

Base centered cubic



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

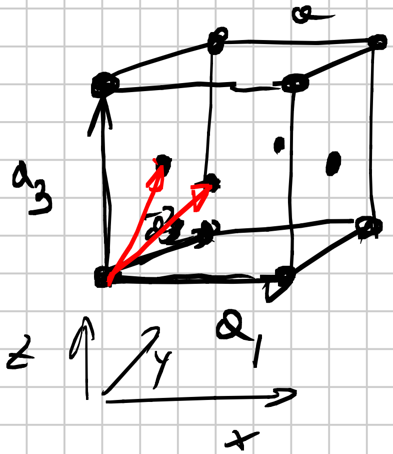
$\vec{a}_2 = (\frac{1}{2}\ \frac{1}{2}\ 0)$

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

BRAVAIS

Side - centered cubic

BRAVAIS ?



$\vec{a}_1$ 1 0 0
$\vec{a}_2$ 0 1 0
$\vec{a}_3$ 0 0 1

Cubic lattice

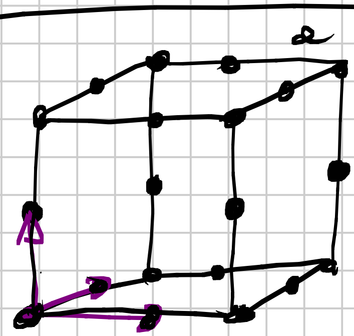
Volume unit cell a^3

$\vec{b}_1 = \left(0 \; \tfrac{1}{2} \; \tfrac{1}{2}\right)$

$\vec{b}_2 = \left(\tfrac{1}{2} \; 0 \; \tfrac{1}{2}\right)$

3 ATOMS on each unit cell

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



Not Bravais

Simple cubic

$a_1 = (1\,0\,0)$
$a_2 \quad (0\,1\,0)$
$a_3 \quad (0\,0\,1)$

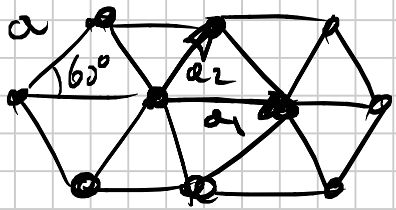
4 atom basis

$\vec{b}_1 \; \left(\tfrac{1}{2}\;0\;0\right) \qquad b_2 \left(0\;\tfrac{1}{2}\;0\right) \qquad b_3 \left(0\;0\;\tfrac{1}{2}\right)$

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

Hexagonal lattice

2D Hexagonal

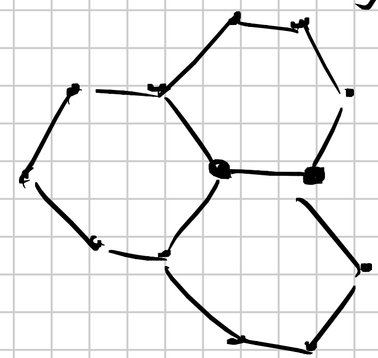


$$\vec{a}_1 = a(1\ 0)$$

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

BRAVAIS LATTICE

[Honeycomb lattice]



NOT BRAVAIS

3D hexagonal

BRAVAIS

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

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

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

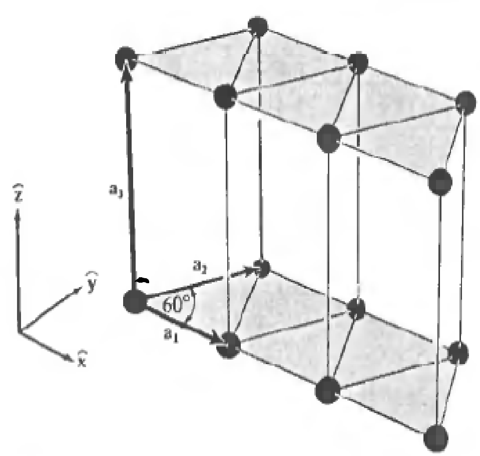
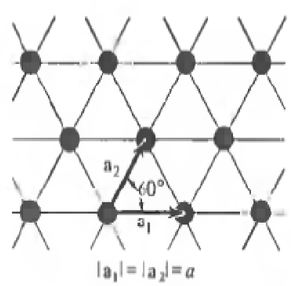


Figure 4.19



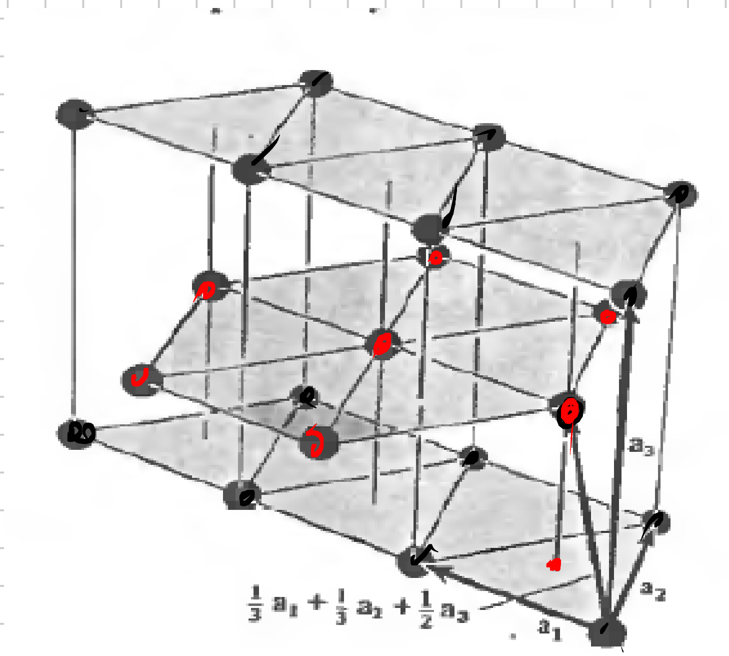
2D

DIAMOND

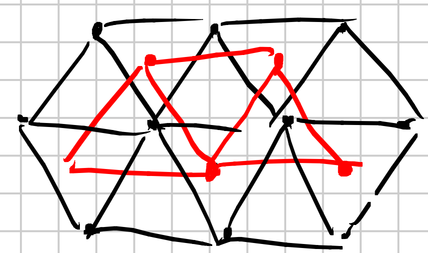
(NOT BRAVAIS) FCC with basis

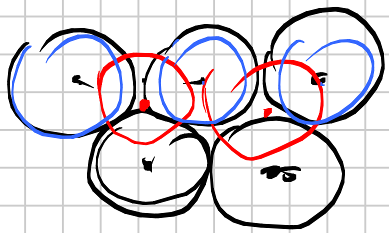
HEXAGONAL LATTICE WITH BASIS

$$\vec{b} = \frac{\vec{a}_1}{3} + \frac{\vec{a}_2}{3} + \frac{\vec{a}_3}{2}$$



HEXAGONAL CLOSE-PACKED

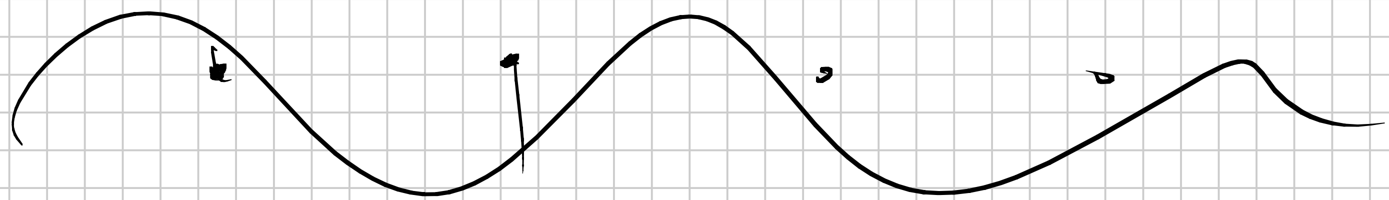




Stack of cannonballs give Hexagonal close packed structure

DIRECT LATTICE (POSITIONS of atoms)

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



Find special K

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

$$\Rightarrow \quad e^{i\vec{K}\cdot\vec{R}_i} = 1 \quad \forall\ \vec{R}_i \text{ in the Bravais Lattice}$$

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

$\{K_i\} \rightarrow$ MAKE A BRAVAIS LATTICE

RECIPROCAL LATTICE

$\{\vec{R}_i\}$ DIRECT BRAVAIS LATTICE

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

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

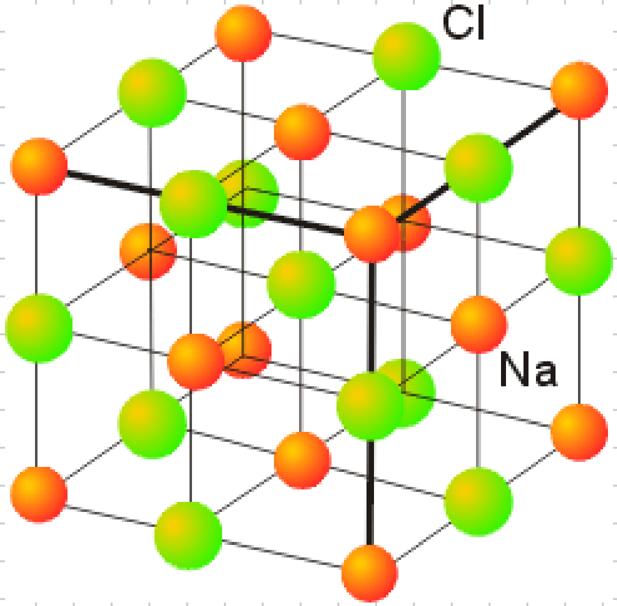
$\Downarrow$

$\{\vec{K}_j\}$ RECIPROCAL LATTICE (BRAVAIS LATTICE)

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

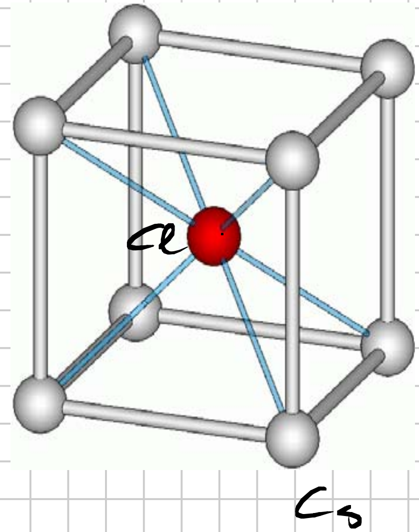
$$\vec{K} = n_1 \vec{b}_1 + n_2 \vec{b}_2 + n_3 \vec{b}_3$$

$NaCl$

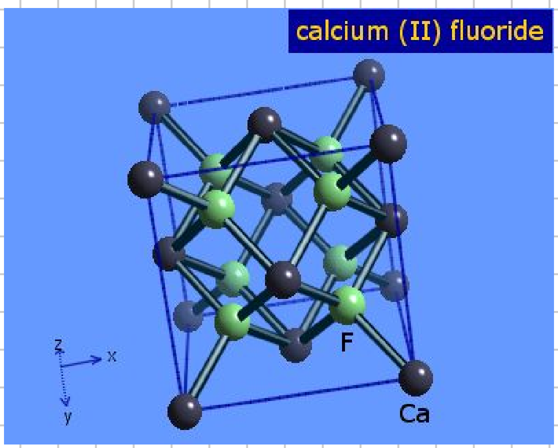


$CsCl$

1



CaF_2



$BaTiO_3$