LECTURE # 10

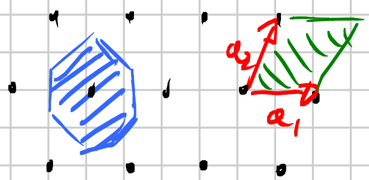
Note Title 2/4/2009

- BRAVAIS LATTICE

$\{\vec{R}_i\}$ $\quad\quad \vec{R}_i = n_1 \vec{a}_1 + n_2 \vec{a}_3 + n_3 \vec{a}_3$ $\quad\quad \vec{a}_i$: PRIMITIVE VECTORS

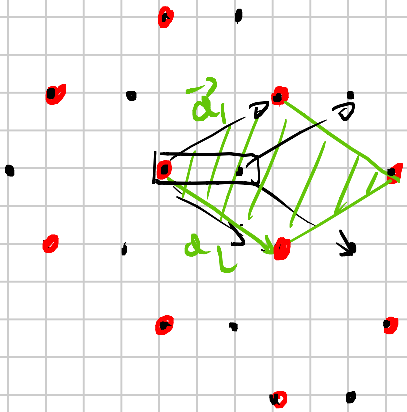
FCC $\quad\quad$ BCC

- UNIT CELL



WIGNER-SEITZ UNIT CELL

"VORONOI" DECOMPOSITION



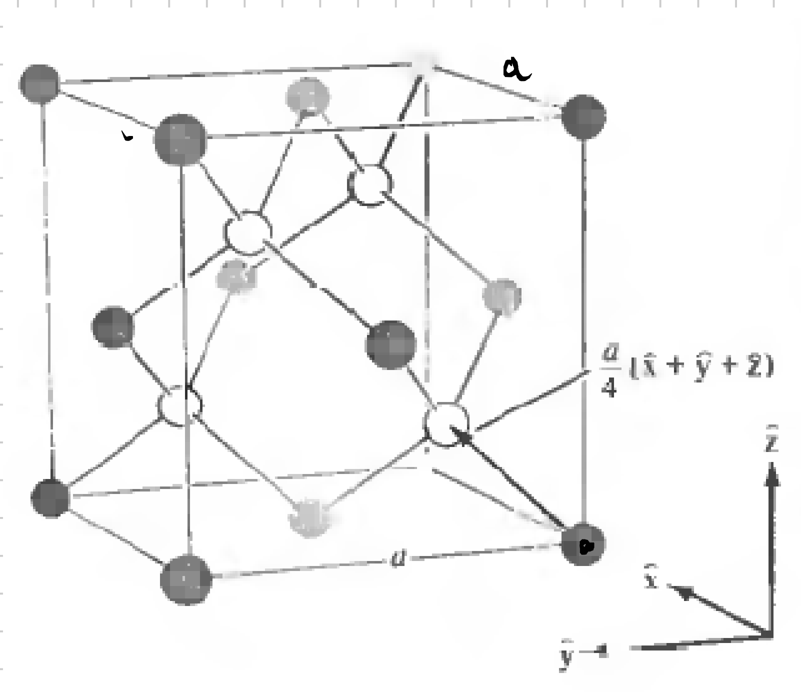
EXAMPLE OF LATTICE WITH BASIS

2 ATOMS / UNIT CELL

→ HONEYCOMB LATTICE

DIAMOND

LATTICE WITH 2- CARBON BASIS



FCC + BASIS

COORDINATES OF 2 CARBONS IN BASIS

Si

Ge

$$\vec{b}_1 = 0$$

$$\vec{b}_2 = \frac{a}{4}(1\ 1\ 1)$$

Ga As ZINC BLEND STRUCTURE

ZnS

HEXAGONAL LATTICE IN 3D

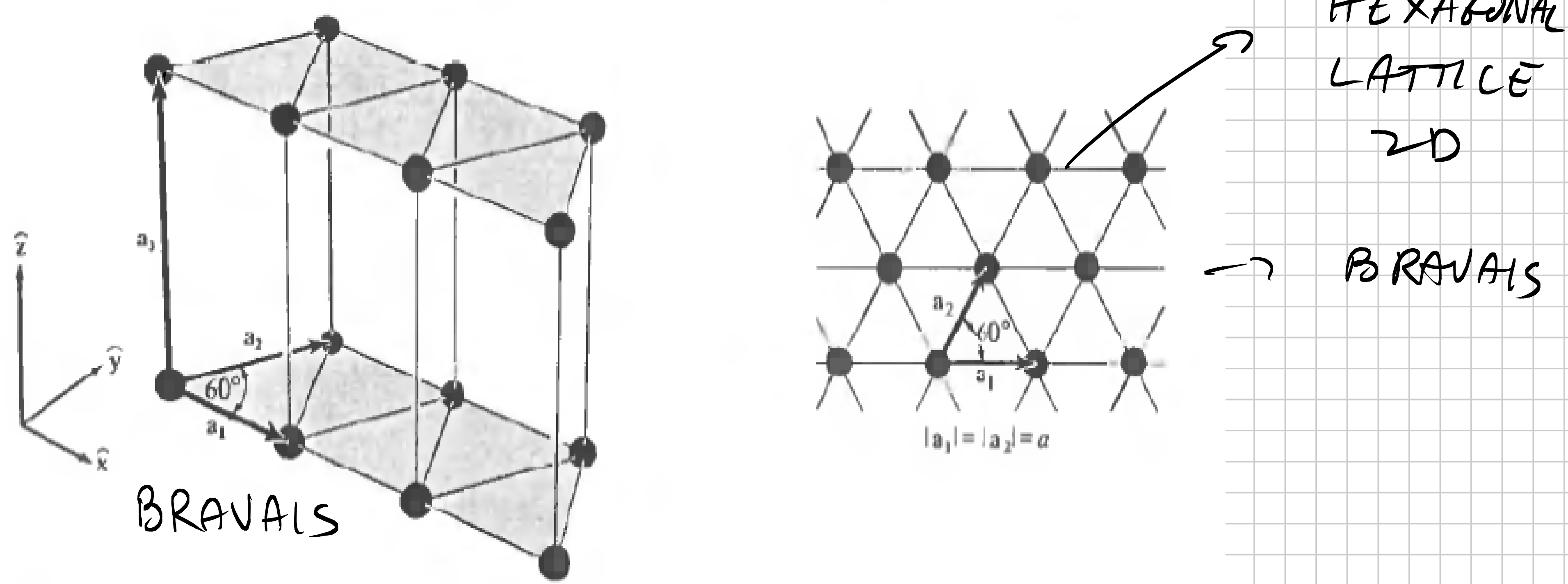
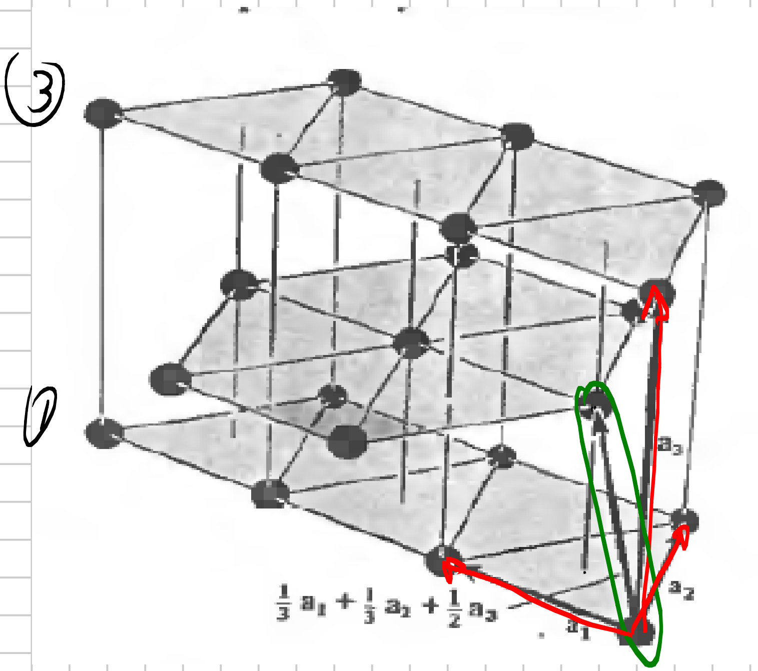


Figure 4.19

HEXAGONAL CLOSED PACKED



$$\vec{b}_1 = 0$$

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

RECIPROCAL LATTICE

REAL SPACE ⟷ WAVE-VECTOR SPACE

DIRECT LATTICES ⟷ RECIPROCAL LATTICE

$f(u)$

$$f(r) = \sum_i \delta(r - R_i)$$

$$f(k) = \int e^{ik\cdot r} f(r)\, dr = \int e^{ik\cdot r} \sum_i \delta(r - R_i)\, dr =$$

$$= \sum_i e^{ik\cdot R_i} \begin{cases} N & k \text{ SUCH THAT } e^{ik\cdot R_i} = 1 \quad \forall R_i \\ 0 & \end{cases}$$

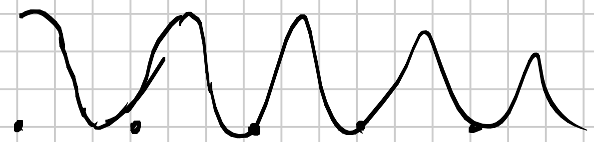
FIND $\underline{K}$ SUCH THAT $e^{i\vec{K}\cdot\vec{R}_i} = 1 \quad \forall R_i$

$\{R_i\}$ BRAVAIS $\Rightarrow$ $\{K_J\}$ AGAIN A BRAVAIS LATTICE

RECIPROCAL LATTICE

$e^{i\frac{2\pi}{a}x}$ $\frac{4\pi}{a}$

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



$e^{i\frac{2\pi}{a(1,1)}x}$

$e^{i\vec{K}\cdot r}$ SHIFT R_i $\longrightarrow$ $e^{i\vec{K}\cdot(r-R_i)} = e^{i\vec{K}\cdot r}\,\cancel{e^{i\vec{K}\cdot R_i}}$

$e^{i\vec{K}_J\cdot\vec{R}_i} = 1$ $\vec{K}_J\cdot\vec{R}_i = 2\pi m$

$\vec{K}_J = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$ $\{\vec{b}_i\}$ PRIMITIVE VECTORS OF RL

GIVEN $\vec{a}_1, \vec{a}_2 \quad \vec{a}_3$ $\qquad b_1 \; b_2 \; b_3$?

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

b_1 ?

$$\begin{cases} \vec{a}_1 \cdot \vec{b}_1 = 2\pi \\ \vec{b}_1 \perp \text{ TO } \vec{a}_2 \text{ AND } \vec{a}_3 \end{cases}$$

$$\vec{b}_1 = c \; \vec{a}_2 \times \vec{a}_3$$

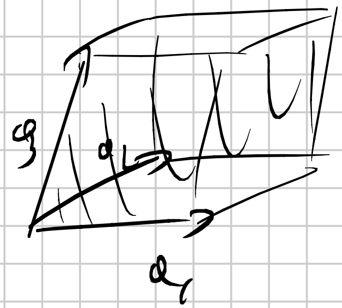
$$c \; \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = 2\pi \qquad c = \frac{2\pi}{|\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|}$$

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

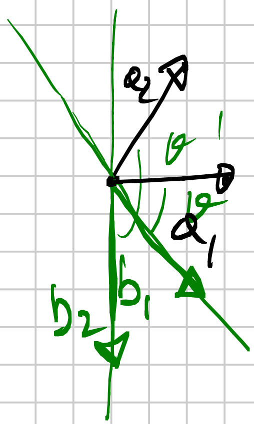
$$\vec{b}_i = \frac{2\pi}{|\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|} \left(\vec{a}_j \times \vec{a}_k \right) \qquad \{i, j, k\} = \{1, 2, 3\}$$

$$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) =$$

VOLUME
OF UNIT CELL



$\boxed{2D}$



$$b_1 \cdot a_1 = 2\pi$$

$$|b_1| = \frac{2\pi}{|a_1| \cos\theta}$$

$$b_2 \cdot a_2 = 2\pi \Rightarrow |b_2| = \frac{2\pi}{|a_2| \cos\theta'}$$

DIRECT

SIMPLE CUBIC

a

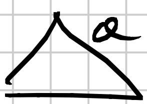
FCC

a

BCC

a

HEX



C DISTANCE
LAYERS

RECIPROCAL

SIMPLE CUBIC

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

BCC

$$b = \frac{4\pi}{a}$$

FCC

$$b = \frac{4\pi}{a}$$

HEX

$$b = \frac{4\pi}{a\sqrt{3}}$$

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