Crystal Lattices - Chpt. 4

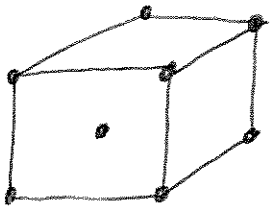
Bravais Lattice: $\{\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3\}$

$\vec{a}$'s = basis

Examples:

Simple cubic: $a\hat{x}, a\hat{y}, a\hat{z}$

Body Centered Cubic: (BCC)



$a\hat{x}, a\hat{y}, \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$

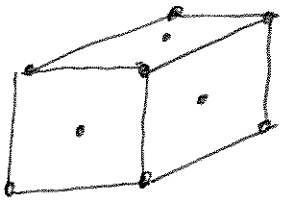
More symmetric:

$$a_1 = \frac{a}{2}(\hat{y}+\hat{z}-\hat{x})$$

$$a_2 = \frac{a}{2}(\hat{z}+\hat{x}-\hat{y})$$

$$a_3 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z})$$

Face Centered Cubic: (FCC)



$$a_1 = \frac{a}{2}(\hat{y}+\hat{z})$$

$$a_2 = \frac{a}{2}(\hat{z}+\hat{x})$$

$$a_3 = \frac{a}{2}(\hat{x}+\hat{y})$$

Coordination number = number of nearest neighbors

6, 8, 12 above

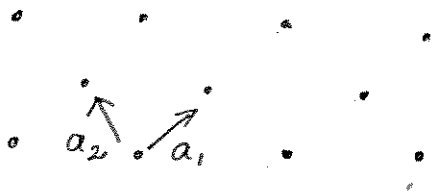
Primitive Unit Cell:

Volume when translated by $\vec{R}$ fills space w/out overlapping. (not unique)

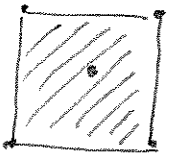
Unit cell:

Fills space when translated by a subset of $\vec{R}$.

2D example:

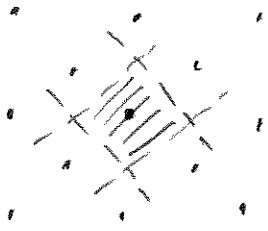


Primitive unit cell 

Unit cell: 

Wigner-Seitz primative cell:

Points closest to a given lattice point:

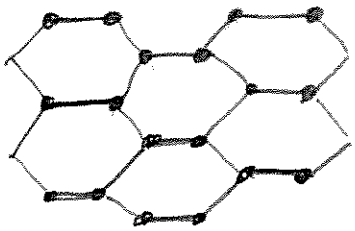


Show 3-D examples.

Lattice w/a basis: $\{\vec{R} + \vec{b}_i\}$

lattice ↑ basis ↑

Examples:



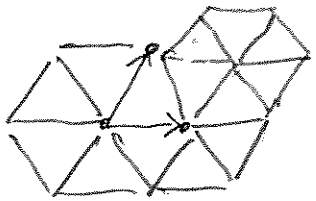
BCC: 2 point basis: $\vec{0}, \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$

FCC: 4 point basis: $0, \frac{a}{2}(\hat{x}+\hat{y}), \frac{a}{2}(\hat{y}+\hat{z}), \frac{a}{2}(\hat{z}+\hat{x})$

Diamond: FCC w/ $\vec{b}_i = \vec{0}, \frac{a}{4}(\hat{x}+\hat{y}+\hat{z})$

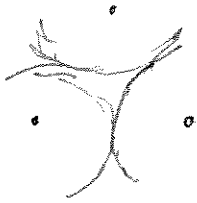
Hexagonal Close-Packed (HCP)

$a_1 = a\hat{x}$, $a_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}$, $a_3 = c\hat{z}$ (simple hexagonal)



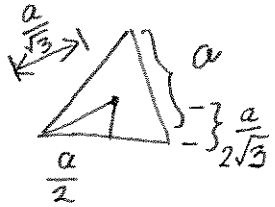
basis $= \vec{0}, \frac{1}{3}\vec{a}_1 + \frac{1}{3}\vec{a}_2 + \frac{1}{3}\vec{a}_3$

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



1 layer

$r = \frac{a}{2}$



∴ Next layer is shifted by:

$\frac{a}{\sqrt{3}}\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right) = \frac{a}{2}\hat{x} + \frac{a}{2\sqrt{3}}\hat{y}$

$= \frac{1}{3}(\vec{a}_1 + \vec{a}_2)$

$\swarrow \frac{a}{\sqrt{3}} + \frac{a}{2\sqrt{3}} = \frac{3}{2}\frac{a}{\sqrt{3}} = \frac{\sqrt{3}}{2}a$ ✓

Third layer shifts back over first layer in HCP.

(tetrahedron)

$$a^2 - \frac{a^2}{3} = h^2 \rightarrow h = \frac{\sqrt{2}}{\sqrt{3}}\, a$$

Since there are two layers,

$$c = 2h = \sqrt{\frac{8}{3}}\, a.$$

We could have also continued to shift (ABC vs. AB). This creates a lattice w/ basis vectors

$$\underbrace{a\hat{x}}_{\vec{a}_1},\ \underbrace{\frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}}_{\vec{a}_2},\ \underbrace{\frac{a}{2}\hat{x} + \frac{a}{2\sqrt{3}}\hat{y} + \sqrt{\frac{2}{3}}a\hat{z}}_{\vec{a}_3}.$$

Note that $|\vec{a}_1| = |\vec{a}_2| = a$ and $|a_3|^2 = a^2\left(\frac{1}{4} + \frac{1}{12} + \frac{2}{3}\right) = a^2$,

and $\vec{a}_1 \cdot \vec{a}_2 = \frac{a^2}{2}$

$\vec{a}_2 \cdot \vec{a}_3 = \frac{a^2}{4} + \frac{a^2}{4} = \frac{a^2}{2}$.

$\vec{a}_3 \cdot \vec{a}_1 = \frac{a^2}{2}$

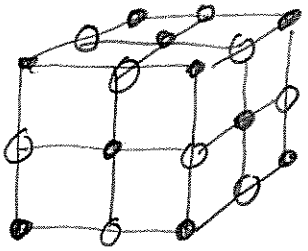
Thus, the vectors each make an angle w/ each other of $\cos^{-1}\left(\frac{1}{2}\right)$. For an FCC lattice we also have

$$\frac{\frac{a}{2}(\hat{y} + \hat{z}) \cdot \frac{a}{2}(\hat{z} + \hat{x})}{\left(\frac{a}{2}\right)^2 \cdot 2} = \frac{1}{2}.$$

Sodium Chloride

FCC w/ basis

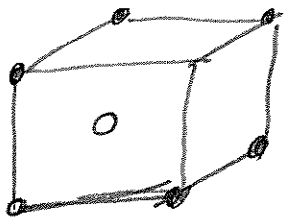
$\vec{0}, \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$



Cesium Chloride

SC w/ basis

$\vec{0}, \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$



Zincblende Structure

Diamond w/ alternating atoms.

Diamond is already a lattice w/ basis.