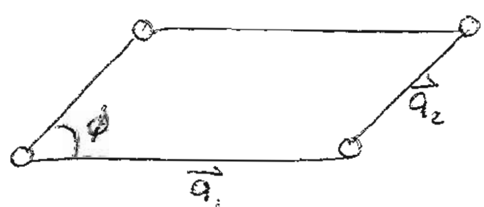
More about Types of Crystal Structures

Bravais lattices are lattices of a distinct type.

There are a finite number of different types of Bravais lattice.

2 - Dimensions

Type 1. most general 2-D lattice = oblique lattice



symmetry = 2-fold
$\Rightarrow$ rotation by $\frac{2\pi}{2} = \pi$
brings lattice into itself

$\boxed{|\vec{a}_1| \neq |\vec{a}_2|}$ ϕ not restricted

by making certain restrictions, we can have
4 other 2-D Bravais lattices

Type 2. square

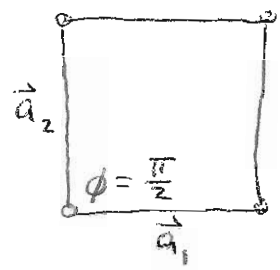
3. hexagonal

4. rectangular

5. centered rectangular

2-D "Bravais" Lattices (Crystal Systems)

2. square : $|\vec{a}_1| = |\vec{a}_2|$; $\phi = 90° = \frac{\pi}{2}$ rad



rot. symmetry = 4-fold

$\Rightarrow$ rotate by $2\frac{\pi}{4} = \frac{\pi}{2}$ brings lattice into itself

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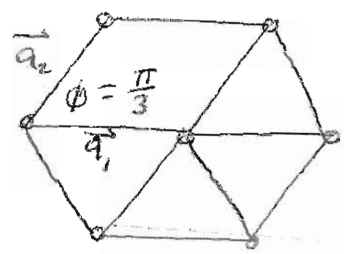
3. hexagonal : $|\vec{a}_1| = |\vec{a}_2|$; $\phi = 60° = \frac{\pi}{3}$



sym: 6-fold

rotate by $\frac{2\pi}{6} = \frac{\pi}{3}$

brings lattice into itself

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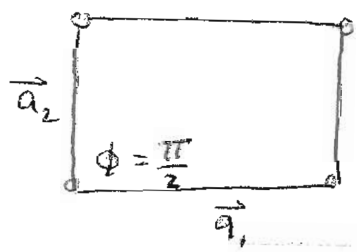
4. rectangular : $|\vec{a}_1| \neq |\vec{a}_2|$; $\phi = \frac{\pi}{2}$



sym: 2-fold

rotate by $\frac{2\pi}{2} = \pi$

brings lattice into itself

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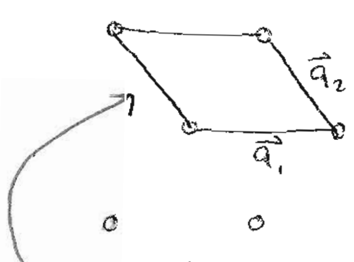
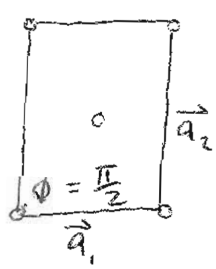
5. centered rectangular : $|\vec{a}_1| \neq |\vec{a}_2|$, $\phi = \frac{\pi}{2}$



or



primitive cell

sym: 2-fold

$\Rightarrow$ rot by $\frac{2\pi}{2} = \pi$

brings crystal into itself

Primitive Cells : 3-D

- contain precisely 1 lattice point

if n is the density of lattice points per unit volume

v is volume of 1 primitive cell

$$\Rightarrow \quad n = \frac{1}{v} \qquad v = \frac{1}{n} \qquad nv = 1$$

this is true for any primitive cell

$\Rightarrow \quad v = \frac{1}{n}$ is the volume of any primitive cell

Primitive Cells: 2-D

- contain precisely 1 lattice point

if σ is the surface density of lattice points per unit area

A is the area of 1 primitive cell

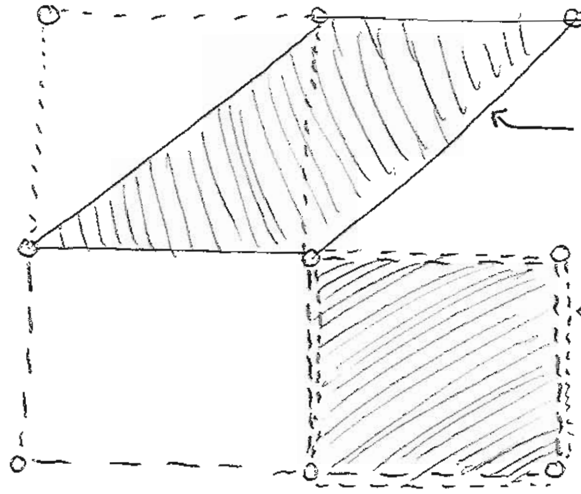
$$\Rightarrow \quad \sigma = \frac{1}{A} \quad \text{or} \quad A = \frac{1}{\sigma} \quad \text{or} \quad \sigma A = 1$$

true for any primitive cell

$\Rightarrow \quad \frac{1}{\sigma}$ = the area of any primitive cell

$\Rightarrow$ different shaped unit cells have same area

2-D Case: example of equivalence of primitive cell area A



area of parallelogram $= A_1$

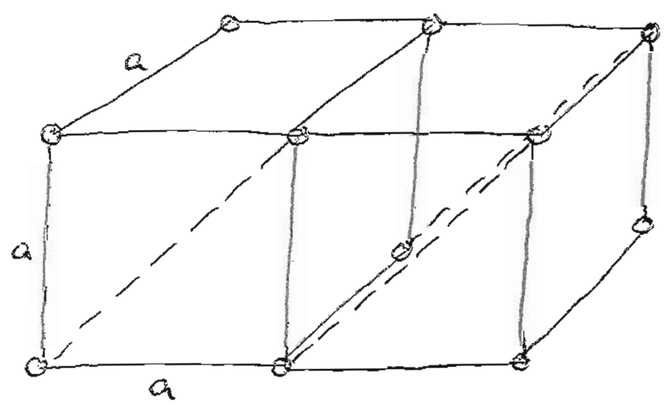
area of square $= A_2$

$$\boxed{A_1 = A_2}$$

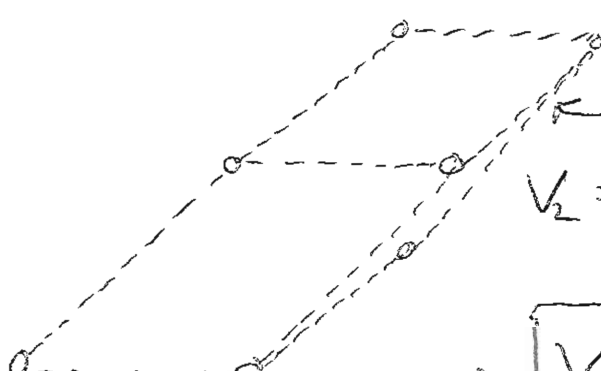
must be true for any choice of the primitive unit cell

3-D

This principle has its analog in 3-D as well



cubical volume $V_1 = a^3$



parallelipiped volume V_2

$$V_2 = \frac{a^3}{2} + \frac{a^3}{2}$$

$$\Rightarrow \boxed{V_1 = V_2}$$

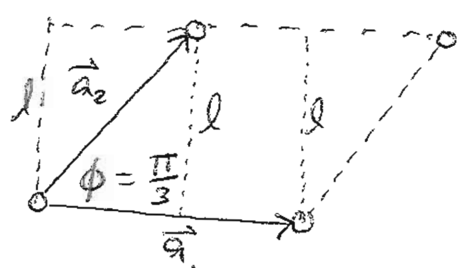
2-D

general way to find the area of the primitive unit cell

- define primitive vectors $\vec{a}_1$ and $\vec{a}_2$
- form the parallelogram bounded by $\vec{a}_1$ and $\vec{a}_2$
- primitive cell is defined having area A

area $\boxed{A = |\vec{a}_1 \times \vec{a}_2|}$

examples: hexagonal lattice



$A = a\,l$

$\vec{a}_1 = a\hat{x}$ $\quad \vec{a}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}$

$$A = |\vec{a}_1 \times \vec{a}_2|$$

$$= |\vec{a}_1| \times |\vec{a}_2| \times \sin\phi = a\, a\sin\phi$$

$$= a \times \left(a \sin\frac{\pi}{3}\right) = a\,l = A$$

3-D

In 3-D this has an analog
general way to find volume of the primitive unit cell

1. define primitive vectors $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$

2. form parallelipiped defined by $\vec{a}_1, \vec{a}_2, \vec{a}_3$

3. primitive cell has volume

$$V = |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|$$

this is obvious for simple cubic in which

$$V = |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|$$
$$= |a\hat{x} \cdot (a\hat{y} \times a\hat{z})|$$
$$= |a\hat{x} \cdot a^2\hat{x}|$$
$$V = a^3$$

For bcc,

$$\vec{a}_1 \times \vec{a}_2 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ a & 0 & 0 \\ 0 & a & 0 \end{vmatrix} = a^2\hat{z}$$

$$V = |(a_1 \times a_2) \cdot \vec{a}_3| = |a^2\hat{z} \cdot \frac{a}{2}(\hat{x} + \hat{y} + \hat{z})|$$

$$\boxed{V = \frac{a^3}{2}}$$

which must be true since bcc has 2 lattice points in one conventional cube of side a

and $V_{prim} = \frac{1}{n}$
$= 1/(2/a^3) = \frac{a^3}{2}$

For fcc

$$\vec{a}_2 \times \vec{a}_3 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{a}{2} & 0 & \frac{a}{2} \\ \frac{a}{2} & \frac{a}{2} & 0 \end{vmatrix}$$

$$= -\frac{a^2}{4}\hat{x} + \frac{a^2}{4}\hat{y} + \frac{a^2}{4}\hat{z}$$

$$V = \left|\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)\right|$$

$$= \left|\frac{a}{2}(\hat{y}+\hat{z}) \cdot \left(-\frac{a^2}{4}\hat{x} + \frac{a^2}{4}\hat{y} + \frac{a^2}{4}\hat{z}\right)\right|$$

$$= \left|\frac{a^3}{8} + \frac{a^3}{8}\right| = \boxed{\frac{a^3}{4}}$$

which must be true since fcc has 4 lattice points per conventional cube of side a

and $V_{prim} = \frac{1}{n} = \frac{1}{4/a^3} = \frac{a^3}{4}$

A problem with the parallelogram (2-D) and parallelopiped (3-D) approaches is that these constructions often lack the symmetry of the lattice

$\Rightarrow$ need for the <u>Wigner-Seitz</u> primitive unit cell method.

(3-D) Bravais Lattices

14 lattice types

Type 1. most general = triclinic lattice

there is 1 sub-type of this type $\Rightarrow$ Number

$$\left.\begin{array}{c} a_1 \neq a_2 \neq a_3 \\ \alpha \neq \beta \neq \gamma \end{array}\right\} \quad 1$$

Type 2. monoclinic $\to$ impose a restriction — Number

$$\left.\begin{array}{c} a_1 \neq a_2 \neq a_3 \\ \alpha = \gamma = 90^\circ \neq \beta \end{array}\right\} \quad 2$$

Type 3. orthorhombic — Number

$$\left.\begin{array}{c} a_1 \neq a_2 \neq a_3 \\ \alpha = \beta = \gamma = 90^\circ \end{array}\right\} \quad 4$$ sub-types

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Type 4. tetragonal

$$\left.\begin{array}{c} a_1 = a_2 \neq a_3 \\ \alpha = \beta = \gamma = 90^\circ \end{array}\right\} \quad 2$$

(st)
(bct or fct) $\to$ just ct

Type 5. cubic

$$\left.\begin{array}{c} a_1 = a_2 = a_3 \\ \alpha = \beta = \gamma = 90^\circ \end{array}\right\} \quad 3$$

(sc)
(fcc)
(bcc)

Type 6. trigonal

$$\left.\begin{array}{c} a_1 = a_2 = a_3 \\ \alpha = \beta = \gamma < 120^\circ, \neq 90^\circ \end{array}\right\} \quad 1 \text{ subtype}$$

Type 7. hexagonal

$$\left.\begin{array}{c} a_1 = a_2 \neq a_3 \\ \alpha = \beta = 90^\circ \\ \gamma = 120^\circ \end{array}\right\} \quad 1$$