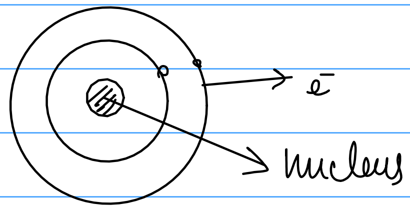
# Solid of Structure

Quantum numbers!

① principal: $n = 1, 2, 3, \ldots$

K shell, L, M




② Azimuthal (subshell) $l = 0, 1, 2, \ldots n-1$

s, p, d ...

$n(\text{protons}) = z = n(e^-)$

Each shell has $n$ subshells.

③ Magnetic

→ Angular $m_l = -l, -l+1, \ldots, 0, 1, \ldots l-1, l$

→ spin $m_s = \frac{1}{2}, -\frac{1}{2}$

④ Spin $s = \frac{1}{2}$

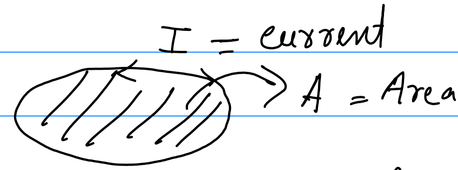
Each shell can accomodate $2n^2$ $e^-$

| | | |
|---|---|---|
| $n=1$ | K shell | 2 |
| $n=2$ | L shell | 8 |
| $n=3$ | M shell | 18 |
| $n=4$ | N shell | 32 |

each subshell can accomodate $2(2l+1)$ $e^-$

| | | |
|---|---|---|
| $l=0$ | s | 2 |
| $l=1$ | p | 6 |
| $l=2$ | d | 10 |
| $l=3$ | f | 14 |

Magnetic moment $\mu = IA$




$A = \pi r^2$ $\quad I = e\nu$ $\quad \nu$ = frequency

both due to spin and orbit angular momentum.

$s$ $\quad l$

$l$ & $s$ can affect one another : L-S coupling
affecting the resultant angular momentum

Total angular momentum $= j = l \pm s$

$= l \pm \frac{1}{2}$ for an $e^-$

for $l = 0$ $j = \frac{1}{2}$

$l = 1$ $j = \frac{1}{2}, \frac{3}{2}$

In case of multi-electron atoms:

method 1 $\left\{ \begin{array}{l} L = l_1 + l_2 + \dots \\ S = s_1 + s_2 + \dots \\ J = L + S \end{array} \right.$

$l_i$ = $l$ of each electron
$s_i$ " s "

method 2 $\left\{ \begin{array}{l} \text{calculate } j_i \text{ for each electron} \\ J = j_1 + j_2 + \dots \end{array} \right.$

92 → natural elements, rest → lab made

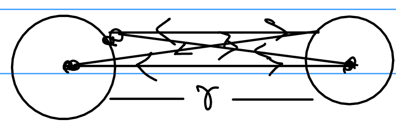
inter-atomic distance

| | |
|---|---|
| solid | 2-4 Å |
| liquid | 5 - 10 Å |
| gas | ~30 Å |

1 mole: $N_A = 6.023 \times 10^{23}$ no. of atoms.

$1\,L = 10^3\ cm^3$

Solid: electrostatic force holds them together.




$e^-$ - nucleus attraction
$e^-$ - $e^-$ repulsion
nucleus - nucleus repulsion.

Net force $\propto \frac{1}{r^n}$

Force $F(r) = \frac{A}{r^m} - \frac{B}{r^n}$  $n > m$

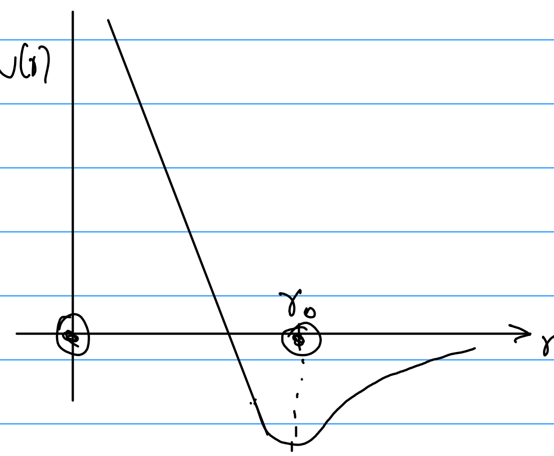
A, B, m, n depends on the nature of atoms.

Potential energy, $U(r) = \int F(r)\,dr$

$$= -\frac{a}{r^{m-1}} + \frac{b}{r^{n-1}}$$

Equilibrium at minimum $U(r)$, at $r = r_0$

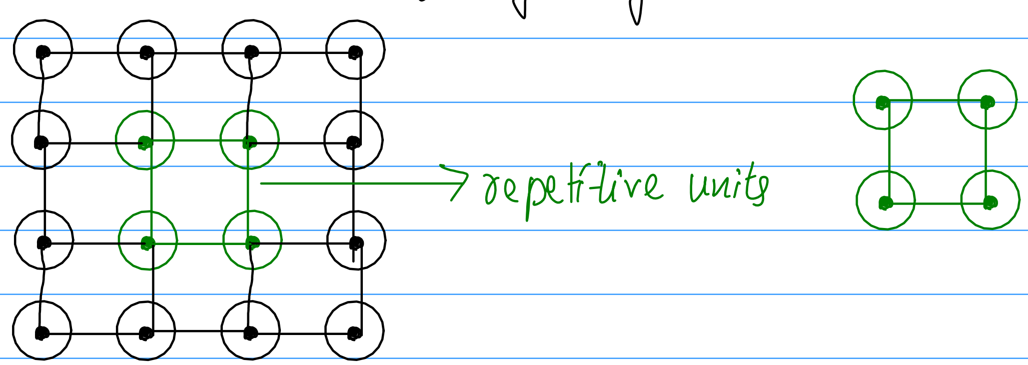
when $\frac{dU(r)}{dr} = 0$




$$\frac{(m-1)a}{r^m} = \frac{(n-1)b}{r^n}$$

$$r_0 = \left(\frac{n-1}{m-1}\,\frac{b}{a}\right)^{\frac{1}{n-m}}$$

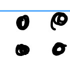
arrangent of atoms in solid



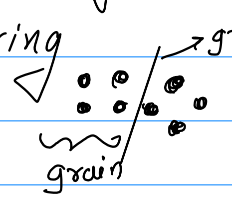

Structure-wise → Crystalline → orderly arrangement of atoms.

Structure-wise → Amorphous → e.g. glass.
↳ randomly arranged atoms

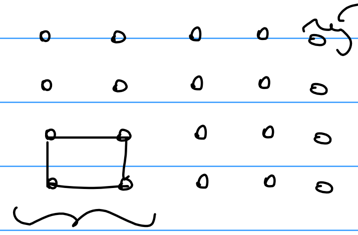
Crystalline → Single → long-range ordering



Crystalline → Poly → short-range ordering

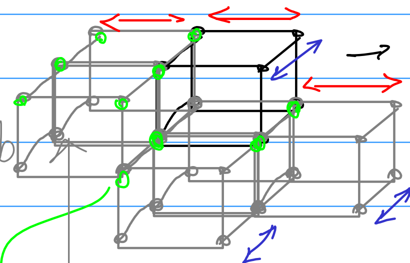


# Bravais Lattice

- Infinite arrangement of points,
- Surrounding of any point is same as that of any other point in the lattice
- The points are called "lattice points"
- 

called "point lattice" or "space lattice"

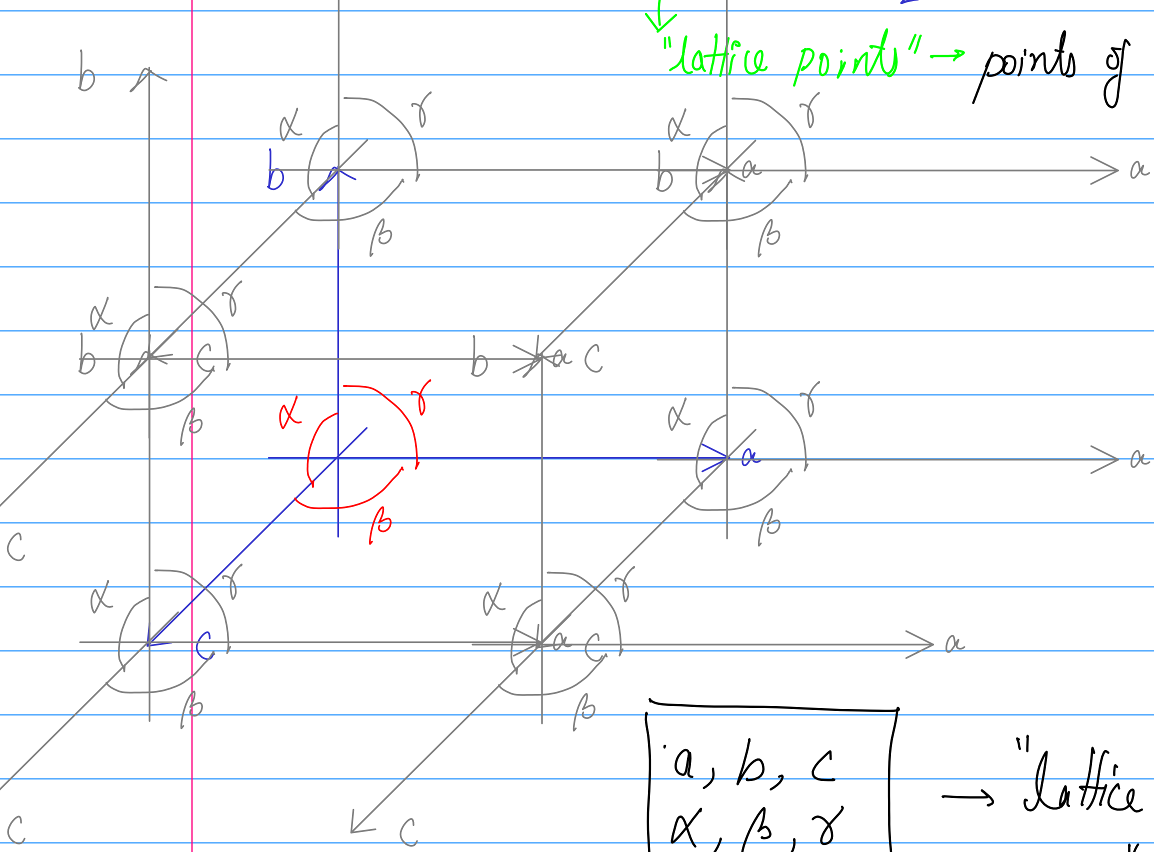
"unit cell"



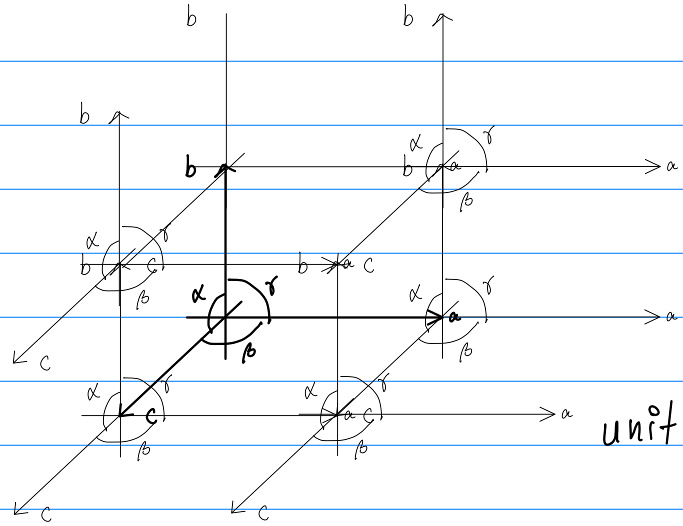
→ 3D unit cell

→ equally spaced parallel planes

"lattice points" → points of intersection of parallel planes



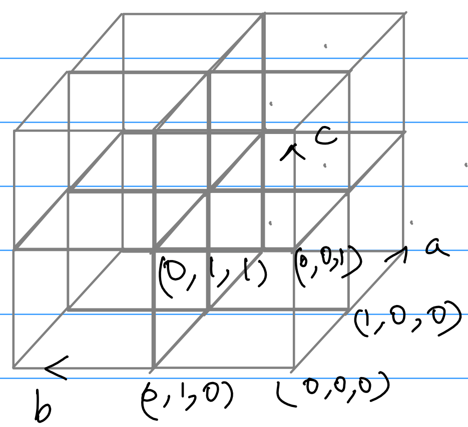

$$\boxed{\begin{matrix} a, b, c \\ \alpha, \beta, \gamma \end{matrix}}$$ → "lattice parameters" or "lattice constants"




unit cell

To generate a space lattice → translation vector $T$

$$T = l\bar{a} + m\bar{b} + n\bar{c} \qquad l, m, n \in 0, 1, 2, \ldots$$




1. $a = b = c$ Cubic lattice
$\alpha = \beta = \gamma = 90^\circ$

2. $a = b \neq c$ Tetragonal lattice
$\alpha = \beta = \gamma = 90^\circ$

3. $a \neq b \neq c$ Orthorhombic lattice
$\alpha = \beta = \gamma = 90^\circ$

4) $a = b = c$ Trigonal lattice

$\alpha = \beta = \gamma \neq 90^\circ$ (Rhombohedral)

5) $a = b \neq c$

$\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$ Hexagonal lattice

6) $a \neq b \neq c$ Monoclinic lattice

$\alpha = \gamma = 90^\circ \neq \beta$

7) $a \neq b \neq c$ Triclinic lattice

$\alpha \neq \beta \neq \gamma \neq 90^\circ$

- The points could be either in corners of the cell (simple), body-centered, face-centered and/or base-centered

- A total of 14 lattice → Bravais lattice