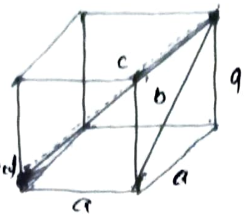
# Cell Calculation

(4)

Once we understand the structure of crystals, we can do many different type of calculations using this information. The calculation involving monoatomic (metallic) cubical ~~system~~ crystal structures.

The Geometry of a Cube.



Where
$a$ = Sidelength of the cube
$b$ = Face Diagonal length
$c$ = Body diagonal length.

using standard trigonometric relationships

$b^2 = 2a^2$,

$c^2 = 3a^2$

$b^2 = a^2 + a^2 = 2a^2$

$\therefore b = \sqrt{2} \cdot a$

$c^2 = 3a^2$

$\therefore c = \sqrt{3} \cdot a$

Thus if we are dealing with a body Centred Cubic structure The body diagonal is the only cell direction that is simple multiple of atomic radii.

Here, we see that $c$ is equal to four atomic radii

$C = 4 \cdot r$.

$r = \frac{c}{4}$

By the same logic, in the face Centred Cubic structure, the face diagonal would be equal to 4 times the atomic radius.

$b = 4r$

or, $r = \frac{b}{4}$

A few simple cubic cells for close packed structures but there are other structures that also fit in a cubic cell structure. For example, diamond has 8 atoms inside a cubic unit cell. NaCl has a f.c.c. structure (of 4 Cl ions) with the $Na^+$ ions in the Octahedral holes (1:1) ratio so since FCC has 4 $Na^+$ ions in each unit cell too.

## Calculation Of Dimensions Of Unit Cell

The dimensions of Unit Cell of a Crystal are.

Edge length of unit cell $= a$
Density of Solid Crystal $= d$
Atomic mass of Solid $= A$

Number of atoms in Unit Cell $= Z$
& Avogadro's Number $= N$

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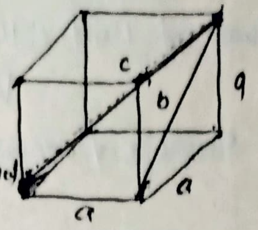


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Let us Consider that-

Edge length of the unit cell of a Cubical Crystal = a

Density of solid Crystal = d

& Mass of One atom of unit cell of (solid Crystal) = m

so, Volume of Unit Cell = $a^3$

$\therefore V = a^3$

Mass of Unit Cell = Number of atoms in Unit Cell × Mass of One atom

Mass of Unit Cell = $Z \times m$

Mass of one atom of unit cell 'm' = $\frac{\text{Atomic Mass}}{\text{Avogadro's Number}}$

$$m = \frac{A}{N}$$

$\therefore$ Mass of Unit Cell = $Z \times m$

$$= Z \times \frac{A}{N}$$

Density of Unit Cell 'd' = $\frac{\text{Mass of Unit Cell}}{\text{Density of Unit Cell}}$

$$'d' = \frac{Z \times m}{a^3}$$

$$'d' = \frac{Z \times A}{a^3 \times N}$$

[The density of unit Cell is the density of Solid Crystal]

$$'d' = \frac{Z \cdot A}{a^3 \cdot N}$$

Density = $\frac{\text{Number of atoms in unit cell} \times \text{Atomic Mass}}{\text{Volume of unit cell} \times \text{Avogadro's Number}}$

$$d = \frac{Z}{a^3} \cdot \frac{A}{N}$$

$$= \frac{Z}{N} \cdot \frac{A}{a^3} = \frac{Z}{N} \cdot \frac{A}{V}$$

Density of Unit Cell 'd' : $\frac{n \times M}{(a^3 . N_A)}$

If M is in grams and a is in c.m then density g/cm³

In Case of Molecules

'n' is the number of Molecules per unit Cell and M is Molar mass.

$$'d' = \frac{n \times M}{a^3 N_a}$$

(Density)