Ac

SHP175 / 502 / C-12

14.09.2021

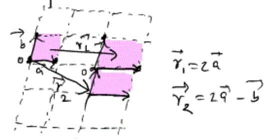
Symmetry operation

[This is an operation which transform the crystal to itself.]

(i) Translation operation.

"motif"

a group of atoms/molecules under symmetry operation to give rise of the crystal structure.



$\vec{r}_1 = 2\vec{a}$

$\vec{r}_2 = 2\vec{a} - \vec{b}$

$\boxed{\vec{r}\,' = \vec{r} + \vec{T}}$

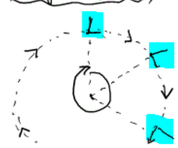
$\Rightarrow \vec{r} = \vec{r}\,' - \vec{T}$

Translated position of the motif.

(ii) Rotation operation

if rotation of the motif by same angle (ϕ) about some axis transforms the lattice to itself

By default;



under 2π rotion lattice remains invarient.

ϕ will be the angle of rotation for sym. operation: iff

2π should be integral multiple of ϕ

$2\pi = n\phi$

$\Rightarrow \phi = \frac{2\pi}{n}$

[if $\phi \leq 2\pi$]

$n \rightarrow$ multiplicity of the axis of rotation.

Reflection

inversion

Rotational sym (continued...)

in general : $n = 1, 2, 3, 4$ and 6

1-fold symmetry, 2-fold symmetry, 3-fold sym, 4-fold sym., 6-fold sym.

$n = 1 : \phi = 2\pi$

$n = 2 : \phi = \pi$

$n = 3 : \phi = \frac{2\pi}{3}$

$n = 4 : \phi = \pi/2$

$n = 6 : \phi = \frac{\pi}{3}$

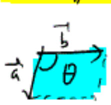
Q: Show that a lattice can't possess a 5-fold symmetry.

— do it as a homework —

Different lattice

2D lattice

Oblique



$|\vec{a}| \neq |\vec{b}|$

$\theta \neq 90^\circ$

invarient under $\phi = \frac{2\pi}{1}$

$\phi = \frac{2\pi}{2}$

$\phi = \frac{2\pi}{3}$

$\phi = \frac{2\pi}{4}$

$\phi = 2\pi/6$

Square

$|\vec{a}| = |\vec{b}|$

$\theta = 90^\circ$

invarient under $\phi = \frac{2\pi}{4}$

Hexagonal

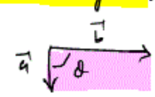
$|\vec{a}| = |\vec{b}|$

$\theta = 120^\circ$

(Otherwise it can't be a part of regular hexagon)

invarient under $\phi = \frac{2\pi}{6}$

Rectangular

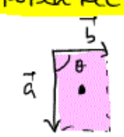


$|\vec{a}| \neq |\vec{b}|$

$\theta = 90^\circ$

it is invarient under reflection

Centered Rectangular



$|\vec{a}| \neq |\vec{b}|$

$\theta = 90^\circ$

it is invarient under inversion operation.

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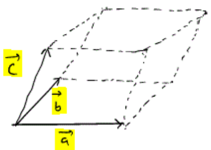
SHPHS / 502 / C-12
15.09.2021 + 21.09.2021

3D (14 types) of lattices are there

↓

Bravais lattice

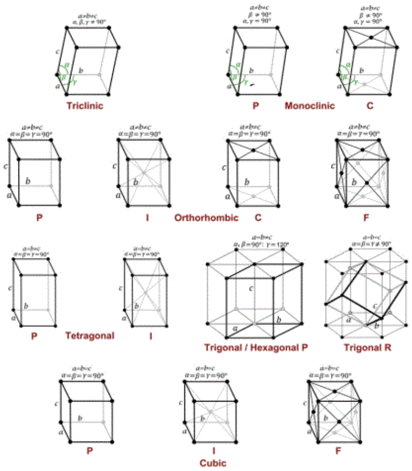
primitive lattice vectors : $\vec{a}$, $\vec{b}$ and $\vec{c}$



$\angle$ bet $\vec{a}$ and $\vec{b}$ = γ
$\angle$ bet $\vec{b}$ and $\vec{c}$ = α
$\angle$ bet $\vec{c}$ and $\vec{a}$ = β

Depending upon $\vec{a}, \vec{b}, \vec{c}$ and (γ, α, β) there are 14 3D space lattice are there. These are called Bravais lattice.

Cubic	Tetragonal	Hexagonal	Rhombohedral	Orthorhombic	Monoclinic	Triclinic
$a=b=c$, $\alpha=\beta=\gamma=90°$	$a=b\neq c$, $\alpha=\beta=\gamma=90°$	$a=b\neq c$, $\alpha=\beta=90°$, $\gamma=120°$	$a=b=c$, $\alpha=\beta=\gamma\neq 90°$, $\alpha=\beta=\gamma(<120°)$ (Trigonal)	$a\neq b\neq c$, $\alpha=\beta=\gamma=90°$	$a\neq b\neq c$, $\alpha=\gamma=90°\neq\beta$	$a\neq b\neq c$, $\alpha\neq\beta\neq\gamma$
→ sc (P) 1	→ st (P) 4	→ sh (P) 6	→ sr (R) 7	→ so (P) 8	→ sm (P) 12	→ st (P) 14
→ fcc (F) 2	→ bct (I) 5			→ fco (F) 9	→ b'cm (C) 13 (base centered)	
→ bcc (I) 3				→ bco (I) 10		
				→ b'co (C) 11 (base centered)		



Atoms per unit cell / number of lattice points in a unit cell

Ex: Cubic system

$$N = N_I + \frac{N_F}{2} + \frac{N_C}{8} + \frac{N_S}{4}$$

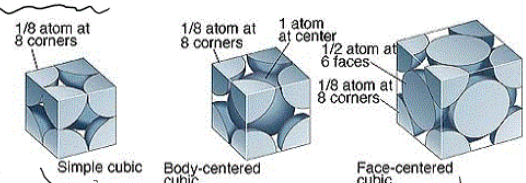
N → Total/effective number of atoms in a unit cell

N_I → no. of atoms completely inside the cell

N_F → no. of atoms at the face

N_C → no. of atoms at the corners

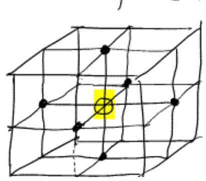
N_S → no. of atoms at any side edge of the unit cell



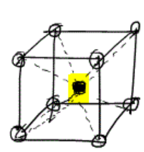
→ Example for Cubic systems.

Coordination number

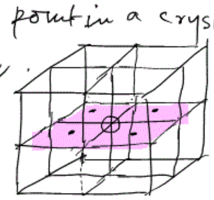
The number of nearest neighbours to an atom or lattice point in a crystal structure.



sc : 6



bcc : 8



fcc : 12
↓
(= 4 × 3)

Q: Show that: $P.F.)_{fcc} > P.F)_{bcc} > P.F)_{sc}$

Q: Show that: $f = 52\%$ for sc, $f = 68\%$ for bcc, $f = 74\%$ for fcc } Here 'f' is the packing fraction.

Hint:

$$f = \frac{\text{Volume of the atoms inside a unit cell}}{\text{Volume of the unit cell.}}$$

$$= 0\cdot****$$

$$\therefore f(\%) = (0\cdot****) \times 100 = **\cdot**$$

Q: Find that lattice const 'a' for a bcc crystal $= a = \left[\frac{2M}{\rho N}\right]^{1/3}$ [H.W]

Q: Find the relation between lattice constant and density of a crystalline material.

Hint: in 1 mole, N no. of atoms are there

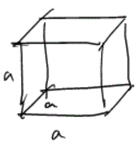
mass of N no. of atom $= M$

" " 1 " " " $= \frac{M}{N}$

" " n " " " $= \frac{M}{N} n$

$$V = \frac{\text{mass}}{\text{density}} = \frac{\frac{Mn}{N}}{\rho} = \frac{Mn}{\rho N}$$

$a = b = c$ (= a say)



$$V = a^3$$

$$a^3 = \frac{Mn}{\rho N}$$

$n \rightarrow$ no. of atom in the unit cell

$$\Rightarrow a = \left[\frac{Mn}{\rho N}\right]^{1/3}$$

Hint: for bcc: $N = N_I + \frac{N_c}{8} = 1 + 8/8 = 2$

$$\therefore a]_{bcc} = \left[2M/\rho N\right]^{1/3}$$