Simple crystal structures

① NaCl → fcc , each ion is surrounded by 6 n.n. of opposite charge

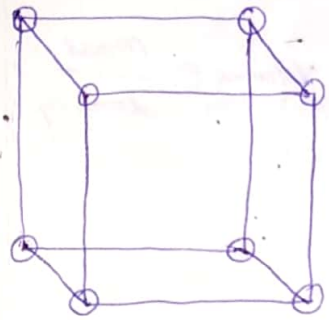
② CsCl → space lattice SC Cs^+ at (0 0 0)

Cl^- at $(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$

Coordination no = 8

③ diamond → Space lattice → fcc

Each atom has 4 n.n & 12 n.n.n



(not complete)

Conventional unit cube contains — 8 atoms.

Lattice consists of two interpenetrating fcc Bravais lattices, displaced along the body diagonal of the cubic cell by one quarter the length of the diagonal. It can be regarded as fcc with two point basis (0,0,0) & $\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})$.

Diamond lattice is not a Bravais lattice.

④ ZnS → lattice is fcc.

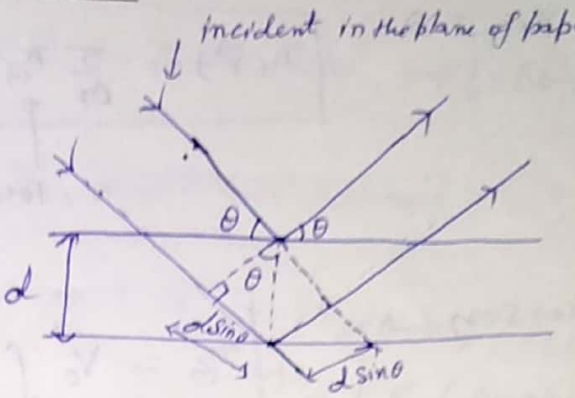
Four molecules of ZnS per conventional cell.

n.n = 4

Cubic ZnS does not have inversion symmetry

ZnS formed when in diamond lattice Zn is put on one fcc lattice and S on other fcc lattice.

Bragg law-



for constructive interference

$2d\sin\theta = n\lambda$

d = spacing of hkl^{th} atomic planes

Condition for Bragg reflection → $\boxed{\lambda \leq 2d}$

Bragg law → consequence of the periodicity of the lattice. It does not refer to the composition of the basis of atoms associated with every lattice point. However composition of basis determines the relative intensity of the various orders of diffraction.

Scattered wave amplitude;—

Fourier analysis —

Any local Physical property is invariant under T as, $\rho(\vec{r})$, $n(\vec{r})$ etc.

Let $n(\vec{r})$ → electron number density

A crystal is invariant under any translation of the form $\vec{T} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$ (u_1, u_2, u_3 → integers)

$n(\vec{r}+\vec{T}) = n(\vec{r})$ → Periodic function of $\vec{r}$, with periods crystal axes
① $\vec{a}_1, \vec{a}_2, \vec{a}_3$ in the direction of three crystal axes.

now ~~$n(x)$ to~~ In 1-D take $n(x)$ with period a in direction x.

F.S. $\therefore$ $n(x) = n_0 + \sum_{p>0}\left[C_p \cos\left(\frac{2\pi p x}{a}\right) + S_p \sin\left(\frac{2\pi p x}{a}\right)\right]$ ——— ②

p = +ve integer
C_p, S_p = real consts

we can show $n(x+a) = n(x)$.

$\frac{2\pi p}{a}$ is a point in the Reciprocal lattice (R.L) or Fourier space

In 1D these points lie on a line.

$n(x) = \sum_p n_p \exp\left(i\frac{2\pi p x}{a}\right)$ p = integer (+ve, zero, -ve)

and n_p = complex number

For $n(x)$ to be real, $n_{-p}^{*} = n_p$

In 3-D

$$n(\vec{r}) = \sum_{G} n_G \exp(i\vec{G}\cdot\vec{r}) \quad \text{——— (3)}$$

Fourier coefficient determines the X-ray scattering amplitude

(3) Inversion →

$$n_G = V_c^{-1} \int_{cell} dV\, n(\vec{r}) \exp(-i\vec{G}\cdot\vec{r})$$

V_c = vol. of a cell of crystal

Reciprocal lattice vectors →

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

$\vec{b}_1, \vec{b}_2, \vec{b}_3$ Primitive vectors of R.L.

$\vec{a}_1, \vec{a}_2, \vec{a}_3$ Primitive vectors of crystal lattice

and, $\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$

Points in R.L. are mapped by set of vectors $\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3$

v_1, v_2, v_3 → integers.

$\vec{G}$ → R.L vector

Every crystal structure has two lattice — Crystal lattice, R.L

Diffraction condition :-

Theorem :- The set of R.L. vectors $\vec{G}$ determines the possible X-ray reflections

For Incident beam Path difference at Points $O, \vec{r}$ is

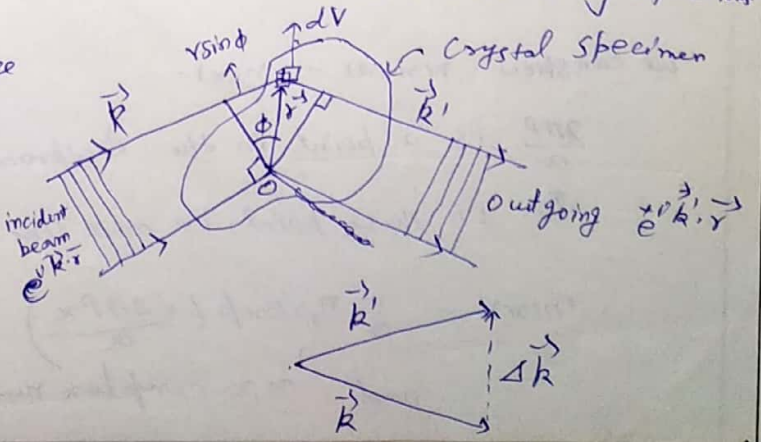
$r\sin\phi$

⇒ Phase difference

$$= \frac{2\pi}{\lambda} r\sin\phi$$

$$= \vec{k}\cdot\vec{r}$$

for diffracted beam → $-\vec{k}'\cdot\vec{r}$



⇒ total difference $= (\vec{k}-\vec{k}')\cdot\vec{r}$

⇒ wave scattered from dV at $\vec{r}$ has phase factor $\exp[i(\vec{k}-\vec{k}')\cdot\vec{r}]$ relative to O.

~~∴ Scattered intensity ∝ amplitude square~~

Total amplitude of scattered wave is $\propto \int n(\vec{r})\, dV \exp[i(\vec{k}-\vec{k}')\cdot\vec{r}$

Say $= F$ (scattering ampli

$$\therefore F = \int dV\, n(\vec{r}) \exp[i(\vec{k}-\vec{k}')\cdot\vec{r}]$$

or $$\boxed{F = \int dV\, n(\vec{r}) \exp(-i\Delta\vec{k}\cdot\vec{r})}$$

Here $\Delta\vec{k} = \vec{k}-\vec{k}'$ $\Delta\vec{r} = \vec{r}'-\vec{r}$

From ③

$$F = \sum_G \int dV\, n_G \exp[i(\vec{G}-\Delta\vec{k})\cdot\vec{r}] \quad \text{—— ④}$$

When $\boxed{\Delta\vec{k}=\vec{G}}$ —— ⑤, $F = Vn_G$

We can show F is negligibly small when Δk differs significantly from any R.L vectors ⇒ ⑤ is diffraction condition

For elastic scattering $|\vec{k}|^2 = |\vec{k}'|^2$

and $\Delta\vec{k} = \vec{G} \Rightarrow \vec{k}+\vec{G} = \vec{k}'$ will give

$$\boxed{2\vec{k}\cdot\vec{G} + G^2 = 0} \quad \text{—— ⑥}$$

$\vec{G}$ is R.L vector ⇒ $-\vec{G}$ also, $\{h, k, l$ may be $-$ve or +ve

$$\boxed{2\vec{k}\cdot\vec{G} = G^2} \quad \text{—— ⑦}$$ Condition for diffraction

∴ For hkl lattice planes d is normal to G and $d_{hkl} = \frac{2\pi}{|G|}$ (show this)

Putting this we get Br in ⑦ we get Bragg law.

Laue Equations :—

Laue equations expresses ⑤ in another way

$\vec{a}_1\cdot\Delta\vec{k} = 2\pi h$, $\vec{a}_2\cdot\Delta\vec{k} = 2\pi k$, $\vec{a}_3\cdot\Delta\vec{k} = 2\pi l$

↓ tell that $\Delta\vec{k}$ lies on a certain cone about the direction of $\vec{a}_1$ and similarly for 2nd & 3rd condition