2D Bravais lattices → 5

square
hexagonal
rectangular
centered rectangular
oblique.

3D Bravais lattices → 14 (From 7 crystal systems)

Monoclinic → 2
triclinic → 1
orthorhombic → 4
cubic → 3
trigonal (rhombohedral) → 1
tetragonal → 2
hexagonal → 1

Cubic lattices

Simple cubic → SC
Body-centered cubic → BCC (E.g Li, Na, K, V, Cr, Fe, Rb, Mo, etc)
Face centered cubic → FCC (E.g Al, Cu, Ni, Ag, Au, Pb, Th, etc)

* Primitive cell of BCC lattice is defined by translational vector,

$\vec{a_1} = \frac{1}{2}a(\vec{x} + \vec{y} - \vec{z})$
$\vec{a_2} = \frac{1}{2}a(-\vec{x} + \vec{y} + \vec{z})$
$\vec{a_3} = \frac{1}{2}a(\vec{x} - \vec{y} + \vec{z})$

* Primitive cell of FCC lattice is defined by translational vectors,

$\vec{a_1} = \frac{1}{2}a(\vec{x} + \vec{y})$
$\vec{a_2} = \frac{1}{2}a(\vec{y} + \vec{z})$
$\vec{a_3} = \frac{1}{2}a(\vec{z} + \vec{x})$

angle between axes are 60°

Note: $\vec{x}$, $\vec{y}$, $\vec{z}$ are cartesian unit vectors.

Note: Hexagonal unit cell is related to the FCC structure.

26/1/2021

LECTURE SLIDES SUMMARY

* A high-temperature superconductor, cooled in liquid Nitrogen, expels local magnetic fields (called the Meissner effect) and causes the magnet to levitate above it.

Classification of solids materials

1) Crystalline (single crystal)
2) Polycrystalline
3) Amorphous.

Note: small single crystal are also called; Crystallites / Grains (domains).

Example of amorphous materials include amorphous silicon, plastics and glasses.

* Growth (and Shapes) of Crystals is determine by,
  1. temperature
  2. pressure
  3. pH (acid or basic environment) etc

Note: Real crystals defects;
(i) surface → (are never perfect)
(ii) Impurities and defects
(3) motion of atoms (lattice vibration)

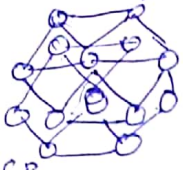
* Ideal crystal → perfect periodicity

Note: Basis are also called motif

* Bravais/crystal lattice → lattice vector
  while Basis → lattice contents

* There is only one lattice point in the primitive unit cells.

ABAB Sequence



HCP

Note: There are little spaces

ABCABC Sequence

FCC or Note: less spaces

*) Both HCP and FCC structures have;

⇒ ideal packing fraction of 0.74

⇒ ideal ratio of c/a for packing as $(8/3)^{1/2} = 1.633$ ($c/a = (8/3)^{1/2}$

*) Wigner-Seitz cell

The Wigner-Seitz cell about a lattice point is the region of space that is closer to that point than to any other lattice point. Wigner-seitz cell is a primitive cell with full symmetry of the Bravais lattice.

It has for S.C, F.C.C, b.c.c

Fivefold rotations and quasicrystals

*) You can only fill space by using rotations of unit cells by; 2π, $\frac{2\pi}{2}$, $\frac{2\pi}{3}$, $\frac{2\pi}{4}$ and $\frac{2\pi}{6}$

i.e (360°, 180°, 120°, 90° and 60°)

$\frac{2\pi}{5}$ or $\frac{2\pi}{n}$ do not fill space

*) A quasicrystals :- Is a quasiperiodic non random assembly of two types of figures (- It is not a Bravais lattice).

Note	Rock salt	perovskite (e.g $BaTiO_3$)	Diamond (Si, Ge) Zincblende (GaAs)
Bravais lattices :	Fcc	cubic	Fcc
position of atom in basis :	O_h		T_d

Elements of Symmetry

Apart from periodicity (i.e translation) each lattice have symmetry properties listed below.

1. Inversion Center
2. Reflection (mirror) plane
3. Rotation axes. only 2-, 3-, 4-, and 6-fold rotations are compatible with translation invariance
4. Rotation - Inversion axes.

1/2/2024

Note: ↓ Ceramic (multi crystalline or polycrystalline)

i) atomic order very among domains or grains but not in polycrystalline material.

ii) Amorphous Silicon can be used in Solar cells and thin film transistors.

Crystal structure = Crystal Lattice + Basis

Note: *) Crystal :- Is a solid with periodic structure.

*) Crystal lattice :- Is periodic array of points. (lattice means Point

*) Crystalline solid :- They are solids in which Component arrangement have long range order.

Unit cell for 2-D → Primitive unit cell (minimum volume)
→ Conventional unit cell

Closed-packed structures

Arrangement of spheres can either be; ABAB or ACAC or any Combination of the two

*) Hexagonal closed-packed (HCP) structure

⇒ Stacking spheres in a ABABAB - configuration

⇒ Atom positions; 000, 2/3 1/3 1/2

⇒ No of nearest neighbours is 12

⇒ Ideal ratio of c/a for this packing is $(8/3)^{1/2} = 1.633$ ($c/a = (8/3)^{1/2}$)

(this value is almost similar to Golden Ratio — assumed for the designing of the pyramids in Egypt)

*) FCC (or Cubic) Called Closed-packed Structure - ccp)

⇒ Stacking arrangement of ABCABCABC ...

Types of bonding

ionic, Vander waals bonding, Metallic bonding, covalent bonding, Hydrogen bonding.

Note: Repulsive interactions between atoms is primarily due to electrostatic repulsion of overlapping charge distributions and pauli principle.

2/2/2021

Lecture 3

X-ray Diffraction

*) X-rays are E-M waves

*) X-rays are scattered by electronic shells (not nuclei) of atoms in a solid.

*) X-rays serve as a bulk probe

The Bragg law

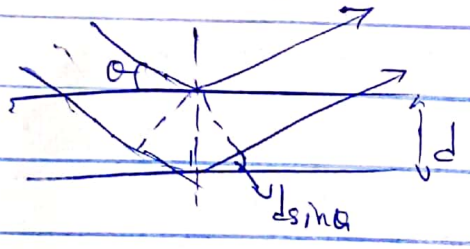
Conditions for peak intensity of scattered radiation:

i) specularly reflection in one plane

ii) Constructive interference of reflected rays.

path difference between two x-rays;

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



Diffraction Grating → Is the tool of choice for separating the colors in incident light.

Meaning of d for 2D → $2d\sin\theta = m\lambda$

Meaning of d for 3D

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

Miller index (say): (111)

$$d_{111} = \frac{n\cdot a}{\sqrt{3}} \approx 3.134 \text{ for Si with } a = 5.43\text{ Å}$$

$$d_{hkl} = \frac{n}{\sqrt{\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}}}$$

Point Symmetry

There are 32 crystal classes (point groups) Combining with translational symmetries, one obtains 230 space groups.

Note: *) Crystal directions; $[n_1 n_2 n_3]$

*) Crystal planes: (hkl)

Miller Indices — represent a set of parallel planes.

Note: Crystal structures are obtained from diffraction experiments (in which particles diffract from planes of atoms).

Note: There are;

i) 7 crystal systems and 14 Bravais lattices

ii) 32 crystal classes (point symmetry groups)

Reciprocal lattice

Given; $T = n_1a_1 + n_2a_2 + n_3a_3$

reciprocal lattice; b_1, b_2, b_3

$$b_1 = \frac{2\pi}{V}a_2 \times a_3,\quad b_2 = \frac{2\pi}{V}a_3 \times a_1,\quad b_3 = \frac{2\pi}{V}a_1 \times a_2$$

Where; $V = a_1\cdot(a_2 \times a_3)$ → vol of unit cell

Note: $b_i a_j = \delta_{ij}$

1) reciprocal lattice to simple cubic lattice — is also a cubic lattice with lattice constant $2\pi/a$

2) reciprocal lattice to bcc lattice — is FCC

also; reciprocal lattice to fcc lattice — is bcc

Brillouin Zone

First Brillouin Zone is the Wigner-Seitz primitive cell of the reciprocal lattice

Lecture 2

Interatomic forces

$$U(R) = -\frac{N\alpha e^2}{4\pi\varepsilon_0 R} + \frac{NA}{R^n}$$

attractive (Coulomb); repulsive

Attractive electrostatic interaction between electrons and nuclei — is the force responsible for cohesion of solids

$F(R) < 0$ for $R > R_0$ → attractive

$F(R) > 0$ for $R < R_0$ → repulsive

$$F(R) = -\frac{\partial V(R)}{\partial R}$$

Note: i) The set of reciprocal lattice vectors determines the possible scattering wave vectors for diffraction.

ii) The reciprocal lattice vector $G = hb_1 + kb_2 + lb_3$ is orthogonal to the plane represented by Miller indices (hkl) → (i.e $V \cdot G = 0$)

iii) The distance (or separation) between two adjacent parallel planes of the direct lattice is,

$$d = \frac{2\pi}{G}$$

iv) Reciprocal vector G (hkl) is normal to crystal plane (hkl) with separation distance; $d = \frac{2\pi}{G}$

Note: Only waves whose wave vector drawn from the origin terminates on a surface of the Brillouin Zone can be diffracted by the crystal.

ii) The BCC and FCC lattices are Fourier transforms of one another.

Experimental X-ray Diffraction techniques

i) White X-ray beam are used for measuring Single crystals → Laue Method

High angular resolution of X-ray diffraction

Normal mismatch ⇒ $\left(\frac{\Delta c}{c}\right) = \frac{\sin w_s}{\sin w_c} \geq 1$

Lecture 4

CRYSTAL DYNAMICS

i) Some properties of atomic motions can be obtained from wavefunction and energies.

Hooke's law

$$F_{spring} = -Kx$$

Angle between two planes

For cubic crystals of; $(h_1 k_1 l_1)$ and $(h_2 k_2 l_2)$ then;

$$\cos\phi = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\ \sqrt{h_2^2 + k_2^2 + l_2^2}}$$

E-1] Calculate the angle btw (111) and (200) planes

Solution

$$\cos\phi = \frac{(1\times2) + (1\times0) + (1\times0)}{\sqrt{1^2+1^2+1^2} \times \sqrt{2^2+0^2+0^2}}$$

$$\phi \simeq 54.75^\circ$$

X-rays and X-ray tube

X-rays are produced when high speed electrons hit the metal target

X-rays and Synchrotons

(Synchrotron radiation → doesn't loss energy but X-ray does)

Natural Synchrotron Radiation → are observed in Stars and galaxies

Synchrotron radiation ⇒ Accelerating electron emits Light

Synchrotron radiation was produced by relativistic electrons in accelerators (since 1947)

$v \simeq 0.9999999c$ $\quad \theta = 4\pi$ srad

$$\theta \simeq \sqrt{1 - \frac{v^2}{c^2}} \simeq 0.001 \text{ srad}$$

Note: i) Synchrotron radiation from a storage ring is the most bright manmade source of white light

ii) useful for materials studies from far infrared and UV to X-rays

Diffraction condition and reciprocal lattice

i) wave vector $|k|$; $k = \frac{2\pi}{\lambda}$

ii) Assumed elastic scattering; scattered X-rays have same energy (same λ) ⇒ same k.

Condition for constructive scattering: ① $(k' - k) \cdot T = 2\pi m$

$k' - k = \Delta k = G$ ⇒ ② $G \cdot T = 2\pi m$

Laue diffraction condition

④ $2d \sin\theta = m\lambda$

③ $2k \cdot G = G^2$ → another expression for diffraction condition

Dispersion relation have two branches!

⇒ Optical Branch → Is due to the +ve sign of root (its called upper branch)

⇒ Acoustical Branch → (Or Lower branch) is due to the -ve sigh of the root.

Note] Dispersion relation ~~for~~ is periodic in K with period T'

$T = 2\pi/a$ (unit cell length)

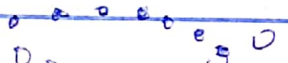
This is true for a chain with arbitary number of atoms per unit cell.

Acoustic/Optical Branches

*) Acoustic branch → give rise to long wavelength vibrations — speed of sound

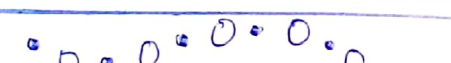
*) Optical branch → is a higher energy vibration.

Transverse optical mode for diatomic chain



N:B Amplitude of vibration is strongly exaggerated!

Transverse acoustical mode for diatomic Chain.



Phonons → Quanta of

lattice vibration. while photons are quanta of ~~E~~ -M wave.

*) Thermal vibrations are thermally excited phonons

*) Sound waves are acoustical phonons

*) ~~Excitations of optical branch~~ Generate optical phonons.

Note] Wave-particle duality holds good for phonons

Sound Waves

*) propagation is through Solids

*) Propagation is governed by the macroscopic elastic properties of the crystal.

Note] Sound waves correspond to ~~the~~ "Low frequency, and long wavelength limit of lattice vibrations."

*) At same f, three sound waves ~~differing~~ can be transmitted, differing in direction of Propagation and velocity.

Speed of Sound wave

$V_L = \lambda\nu = \sqrt{\frac{c}{\rho}}$ c = elastic bulk modulus, ρ = Mass density,

Note] C is inversely related to ρ

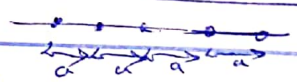
Note] Solids will sustain the propagation of transverse waves, which travel more slowly than longitudinal waves.

Solid	Structure type
⇒ Sodium	BCC
⇒ Copper	FCC
⇒ Aluminum	FCC
⇒ Lead	FCC
⇒ Silicon	Diamond
⇒ Germanium	Diamond
⇒ NaCl	Rocksalt.

Note] Lattice vibrational wave in crystal could be;

- Longitudinal
- Transverse or some combination of the two.

Monoatomic Chain



*) Simplest Crystal is 1D chain

*) Atoms are identical

*) Atoms move in a direction parallel to the chain

*) Only nearest neighbours interact (Short-range forces)

Chain of two types of atom

*) It is the simplest possible model of an ionic Crystal

*) 'a' is repeated distance

*) a/2 is nearest neighbours Separations distance

$E_n = nh\nu = n\hbar\omega_0$

* $\theta_E = \frac{\hbar\omega_0}{k_B}$ → Einstein temperature

Debye assumption

1) Crystals propagate elastic waves of λ ranging from low f (sound waves) to high corresponding to infrared absorption.
2) Dependent ~~vibrat~~ coupled vibration of oscillators.
3) Different f hence different θ.

If resulted into;

$$C_v = 3K\left(\frac{\theta_D}{T}\right)F_D$$

Thermal energy and lattice vibrations

* In solids, vibration and rotation of atoms and molecules contribute to thermal energy
* In gas, translational motion of atoms and molecules contribute to this energy

Note: Thermal energy can be used to activate a crystallographic or a magnetic transition

Heat capacity from lattice vibrations

* Heat capacity of a metal
  = Contribution from; lattice vibration and conduction electrons
* Heat capacity of a magnetic materials
  = ~~Contrib~~ Frgng lattice vibration and magnetic ordering
* Heat capacity of a non-magnetic insulators
  = Contribution from lattice vibration only.

11/2/2021 | LECTURE 5

Energy bands and Semiconductors

* Conduction band is of higher energy than valence band.
* Difference in energy of CB and VB is the Band Gap (or forbidden Gap)

Sound waves → Is the collective modes of dependently vibrating lattices which propagate through a material.

Quantum harmonic oscillators energy;

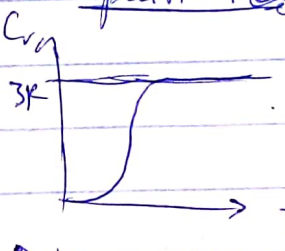
$$\Delta E = h\nu$$

Note: Evidence of vibrational energy in ~~Solid~~ periodic solid is true; energy is quantized (i.e discrete) and called "phonons"

$$E_{phonon} = \frac{h\nu}{\lambda} \quad \lambda \rightarrow \sim 10^{-10}\,m \qquad E_{photon} = \frac{hc}{\lambda} \quad \lambda \approx 10^{-6}\,m$$

$$P_{phonon} = \frac{h}{\lambda} \qquad P_{photon} = \frac{h}{\lambda}$$

Specific heat of solids



At B:
$C_v \cong 3R$ at high temperature

Dulong–Petit law states that
"the specific heat of a given number of atoms of any solid is independent of temperature and is the same for all materials".

$$C = \frac{dQ}{dT} \rightarrow \text{Specific heat}$$

$$C_{solid} = C_{latt} + C_{elec} \quad (C_{elec} \text{ is relatively small})$$

Note: N atom vibrating in 3-D is equal to 3N atom vibrating in 1-D

$$\therefore E = 3NK_BT$$

$$\Rightarrow \boxed{C_v = \left(\frac{\partial E}{\partial T}\right)_v = 3NK_B}$$

Failure of Einstein's theory

1) Oscillators vibrate at same natural frequency hence same energy
2) Independent vibration of oscillators

Fermi-Dirac Statistics / distribution

$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1}$$

- Electrons are fermions
- at $T = 0$, no electrons can move above V.B
- at $T > 0$, some electrons can reach the C.B and contribute to electric current.

PN-junction diode

- They are one way device
- They are used as rectifiers (for converting a.c to d.c)

LECTURE SLIDE 6

Hall Effect (based on charge and voltage)

principles

Discharges

"Lorentz force pressed mobile charges to one side while immobile charges are unaltered"

This creates internal electric potential called Hall voltage

$$V = \frac{IB}{net}$$

Applications

- It gives information about charge carrier mobility and concentration

- Insulator → have large band gap
- Semiconductor → Narrow band gap
- Conductor → No band gap.

Fermi level

- For an intrinsic semiconductor, the fermi level is almost at the middle of the band gap.
- For a p-type extrinsic semiconductor, the fermi level is closer to V.B
- For an N-type it is closer to C.B

NOTE: Metals are good conductors of electricity due to the overlap of V.B and C.B so that V.B electrons can move through the material.

Semiconductor

- E.g → Si and Ge
- They have almost empty conduction band and almost filled valence band with very narrow energy gap

Intrinsic Semiconductor

- No of electrons = No of holes

P-type

Extrinsic S.c

i) N-type
no of electrons > no of holes

ii) p-type
no of holes > no of electrons

NOTE: At absolute temperature (i.e $T = 0$) the highest level electrons can reach is the fermi level with energy called Fermi energy.

NOTE: The essence of doping is to increase the conductivity of semiconductor material

NOTE: i) N-type are formed using pentavalent elements (like Arsenic, Antimony, phosphorus etc) as dopants. N-type dopants are called donors

ii) p-type are formed using trivalent elements (like indium, Boron, Aluminium etc) as dopants. p-type dopants are called acceptors.

iii) Dopants form covalent bonds with the Semiconductor

* It is used in
→ Hall probe
→ in cars
→ in space
→ New Discoveries e.t.
→ Quantum Hall Effect
→ Spin Hall effect
→ Anomalous Hall Effect

Hall coefficients

* It is determined by measuring the Hall voltage that generates the Hall field.