

Day - 19

→ Description of perfect crystals



Characterization of a material — XRD

Starting point → Real crystals



Perfect crystals + defects
introduced in them

→ Dimensionality:

- higher dimensional defects (HD defects)
- 1-D defect
- 0-D defect

line defect

2D: surface

3D: void/pore

point defect

dislocations

crack propagation

observation
in the
crystal
structure
at a location

plastic
deformation
in materials

stress concentration at
a void.

↓
vacancies, interstitials, e^-/h^+

↳ electronic devices

order of size of defect $\geq 1 \text{ nm}/\mu\text{m}$

higher dimensional

$1 \text{ nm}/\mu\text{m} \rightarrow 1\text{D}$ defect

- Point defects
 - ionic
 - electronic

- HD defects \rightarrow interfaces

material and the ambient

broken bonds (at the surface)

internal interfaces

grain boundary

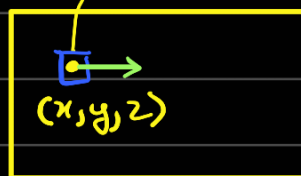
hetero-interface

boundary region
between 2 grains

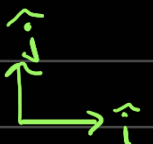
(what is the plane normal?)

sit here

block



assume (hkl)



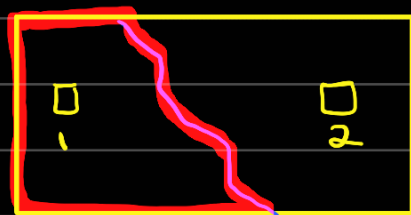
irrespective of (x, y, z)
if O.R. is satisfied,
we get single crystal

orientation
relationship (O.R.)

$$\begin{cases} (hkl) \parallel (xy \text{ plane}) \\ [uvw] \parallel \hat{i} \end{cases}$$
$$hu + kv + lw = 0$$

let at location 1,

$$(h_1 k_1 l_1) \parallel \hat{k}, [U_1 V_1 W_1] \parallel \hat{i}$$



At location 2,
 $(h_2 k_2 l_2) \parallel \hat{k}$
 $[U_2 V_2 W_2] \parallel \hat{i}$

grain

o.r. changes at this boundary
(hinders e^- transfer)

This is a polycrystalline material.

It has a single OoRo.

when there is a unique $(h k l) \parallel \hat{k}$
but $[U V W]$ can be different,
we call the material textured.

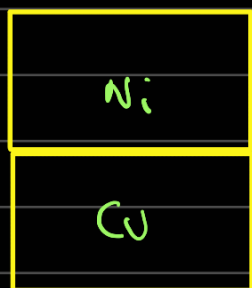
→ Hetero-interface:

Between 2 different materials

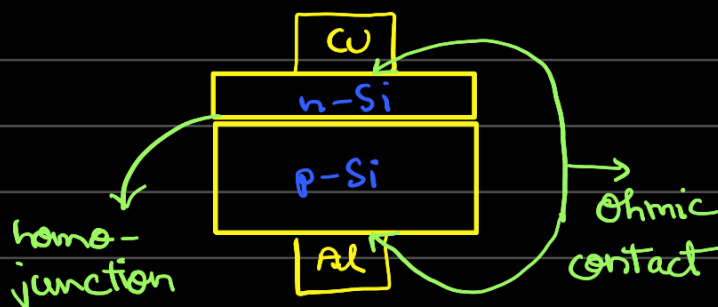


device

(eg: Bimetallic Barring)



p-n juncⁿ diode



→ insulating materials



perovskite



LaAlO_3 , SrTiO_3

Insulators

Tapping the surface → became metallic

metal → 2D electron 'gas'

collection of e^- in metal is modelled as
ideal gas (3D e^- gas)