Defects and Crystal Characterization

Equilibrium Demands Defects (additional data in Wolf, Chapter 2 and Sze Chapter 10)

$$\boxed{\Delta G = \Delta H - T\Delta S}$$

defects are higher enthalpy

but increase entropy (randomness)

$$\boxed{\#\text{ of defects} \uparrow \text{ as Temp} \uparrow}$$

Thermodynamics!

Point defects: (eg. vacancy or interstitial)

At equillibrium:

$$\boxed{N = N_0 \exp\left(-E_A/kT\right)}$$

→ but thermal processing does not usually leave samples in Equillibrium!

defects ⇒ lose some ΔH, but gain some ΔS

E_A for vacancy (Schottky Defects in Si ~ 2.6eV)

$N_0 \sim 5 \times 10^{22}/cm^3$ (atoms per cm^3 for Si)

So at RT (300K) 1 in 10^{34}

↓ vacancy ↓ sites

at 1000K 1 vacancy in 10^{34} sites

Real Crystals are not ideal

Show Figures on laptop/projector.

1. Surfaces → termination, dangling bonds, reconstruction (actually area defects)

2. Point Defects
   a. intrinsic
      i. vacancy (lattice site → surface) : Schottky defect
      ii. interstitial (surface → interstitial site)
      iii. Frenkel defect vacancy - interstitial pair
   b. extrinsic - involve foreign atoms
      - lattice (electronically active - eg. dopants)
      - interstitial (diffuse faster, ie. Cu in Si)

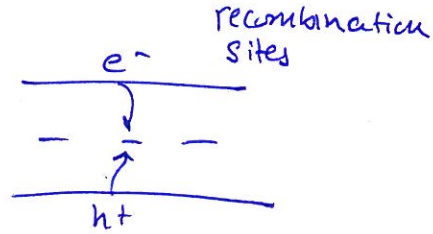
3. Line Defects (see book)
   a. edge dislocation (extra "sheet" of atoms in part of stack)
   b. screw dislocation (shear part of crystal)

   c. area defects
      - twins - change in crystal orientation across a plane
      - grain boundary - transition between crystals w/ no specific orientation relationship.
      - stacking fault - ABCABC
        ABABC
        or ABCCABC etc.

D. volume defects
   - precipitations (agglomeration of defects upon cooling, usually)

Defects and Impurities Cause:

(1) Energy levels in band gap



(2) Defects can trap charge (e.g. reducing carrier concentration)

- # charged defects depends on doping (i.e. position of Fermi level relative to impurity level)

(3) defects can organize upon temperature cycling

(4) Defects Trap impurities (Gettering Sites)

(need more here discussion)

Example: intrinsic impurity gettering in CZ Silicon

(a) high T → "denuded" zone due to outdiffusion

~ 15-18 ppma

~ 12 ppma threshold [O] for precipitation

(b) Low T → nucleation of ~~defects~~ ~~in Bulk~~ SiO clusters in Bulk

(c) high T → growth of clusters

→ dislocation loops surrounding clusters serve as ~~defect~~ ~~gettering~~ ~~impurit~~ impurity gettering sites.