Crystal Defects

(scan Kittel Ch. 18, 20 look at figs.)

• Real crystals are never perfect

• Semiconducting properties of most interest are predominantly caused by crystal defects

Main types of defects:

1. Point defects (single atoms, vacancies)
2. Line defects (dislocations)
3. Plane defects (surfaces, grain boundaries)
4. Volume defects (small inclusions, precipitates, defect clusters)

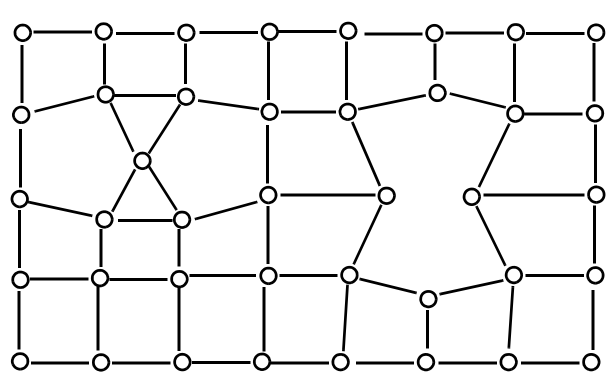
Point defects

• Native defects:

vacancies (missing atom)
interstitials (extra host atom, not on a lattice site)
anti-site defect (e.g. in GaAs, Ga on an As site, or vice-versa)

• Impurities: could be substitutional or interstitial

The lattice surrounding a defect usually relaxes.



From thermodynamics:

Schottky:

y

for diatomic lattice: charge neutrality requires equal #s of anion, cation vacancies

Frenkel (similar to diatomic):

energy to take one atom and put it at a distant interstitial site

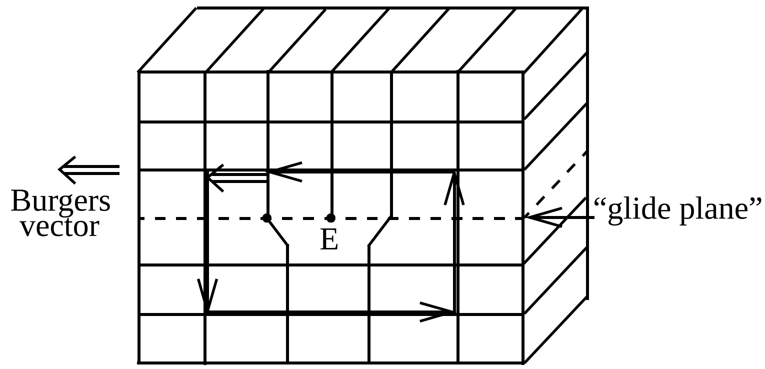
$$N_F = (N_L N_i)^{1/2} \exp\left(\frac{-E_F}{2kT}\right)$$

<u>**Dislocations**</u>

2 types:

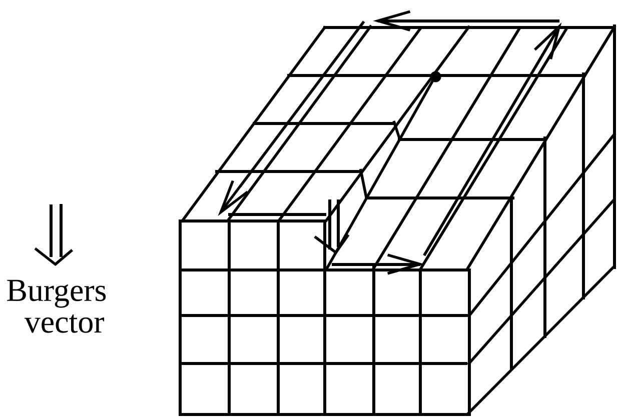
- edge dislocations
- screw dislocations

<u>Edge dislocation:</u> extra lattice plane inserted partway into a crystal



<u>Screw dislocation</u>

- cut crystal partway through
- shear parallel to cut by one atom spacing
- important for crystal growth: maintains a step as crystal grows. Unwanted macroscopic growth spirals may result.



Burgers vector: construct polygon with equal # lattice steps on each side.

- closed in a perfect crystal, around a dislocation, it is not closed.
 Lattice vector needed to close is called "Burgers vector"

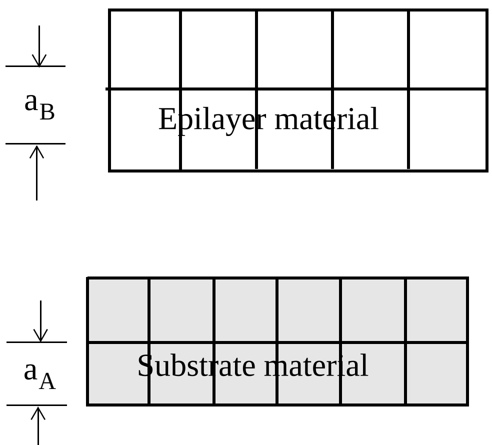
Dislocation lines typically thread to a surface. High densities of dislocations can form closed loops.

Dislocation density is an important measure of crystal quality. Best Si, Ge single crystals $< 1 - 10/cm^2$. Heavily deformed metals $10^{11} - 10^{12}/cm^2$.

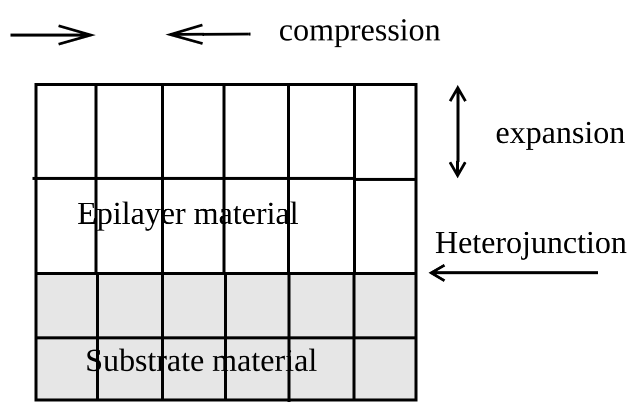
Common quick method for counting dislocations is surface etching:
Parts of lattice surrounding dislocation are under stress. Acid etch is faster here. Creates pits visible in a microscope or even naked eye. Count up to ~ $10^8/cm^2$.

Dislocations are important in hetero-epitaxy

Substrate material A, lattice constant a_A
Epi-layer material B, lattice constant a_B

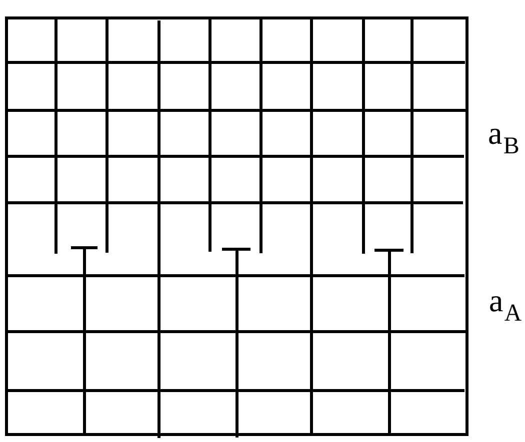


Before growth:
relaxed structures of
both materials



After growth:
commensurate (strained)
epitaxy

with relaxation - misfit dislocations result:



fully relaxed with misfit
dislocation array at
interface

Critical Thickness d_c

for epilayer thickness < d_c , commensurate strained layer epi occurs. For thickness > d_c , strain relaxes by forming mismatch dislocations. Semi-empirical formula for critical thickness:

Burgers vector

$$d_c \cong \frac{a}{\Delta a}\frac{b}{4\pi(1+\nu)}\left\{\ln\left(\frac{d_c}{b}\right)+1\right\}$$

Poisson ratio

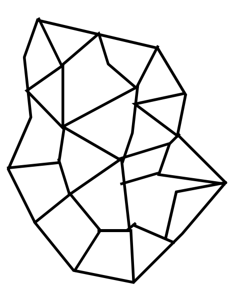
for 2% mismatch, with typical b = 4 Å, ν = 0.3,

Polycrystalline material, grain boundaries

(e.g. poly-silicon) very commonly used for gate material of modern MOSFETS

LPCVD of silicon on SiO2 - random nucleation of crystal ⟶ many randomly oriented "crystallites" or "grains."

grain boundary - interface between grains

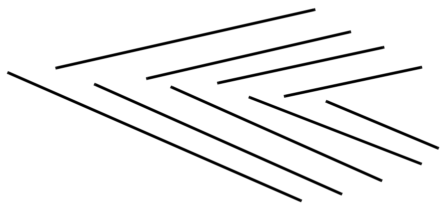


electron transport across grain boundaries related to interface defects.

Also dopant diffusion strongly influenced by grain boundaries.

low angle grain boundary

⟶ array of dislocations



large angle grain boundaries'

⟶ may have irregular, or regular arrays of dislocations