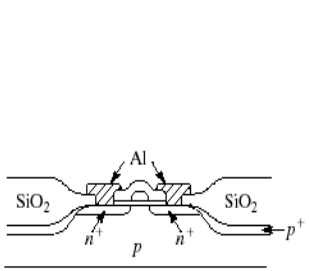
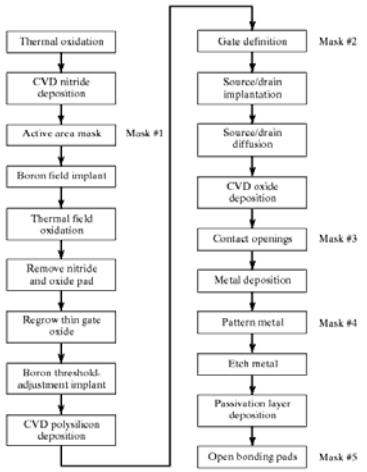
Review: Basic NMOS process flowchart.



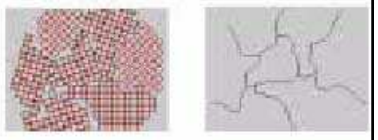


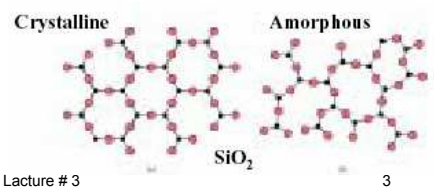
2.2: Crystal structure: **How do atoms arrange themselves to form solids?**

- **Fundamental concepts and language**
- **Unit cells**
- **Crystal structures**
- **Face-centered cubic**
- **Body-centered cubic**
- **Hexagonal close-packed**
- **Close packed crystal structures**
- **Types of solids**
- **Single crystal**
- **Polycrystalline**
- **Amorphous**

Types of Solids

- **Crystalline material**: atoms self-organize in a periodic array
- **Single crystal**: atoms are in a repeating or periodic array over the entire extent of the material
- **Polycrystalline material:** comprised of many small crystals or **grains**
- **Amorphous:** lacks a systematic atomic arrangement





Crystal structure

- To discuss crystalline structures it is useful to consider atoms as being hard spheres with well-defined radii.
- In this hard-sphere model, the shortest distance between two like atoms is one diameter.
- We can also consider crystalline structure as a lattice of points at atom/sphere centers.

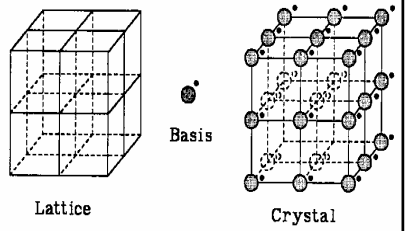
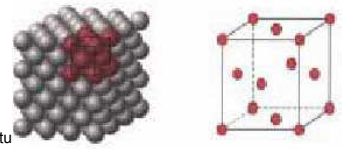
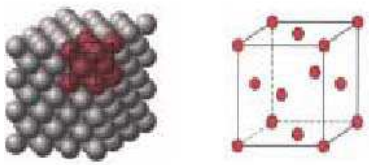


Fig. 1.3 Lattice + basis = crystal structure.

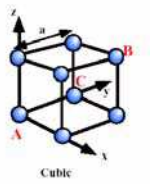


Unit Cell

- The unit cell is the smallest structural unit or building block
- that can describe the crystal structure. Repetition of the
- unit cell generates the entire crystal.
- Example: 2D honeycomb net can
- be represented by translation of
- two adjacent atoms that form a unit cell for this 2D crystalline structure



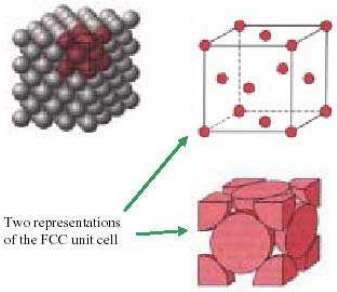
- Different choices of unit cells possible, generally choose
- parallelepiped unit cell with highest level of symmetry

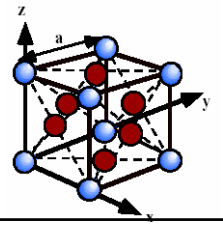


Crystals are characterized by a unit cell which repeats in the x, y, z directions.

Face-Centered Cubic (FCC) Crystal Structure (I)

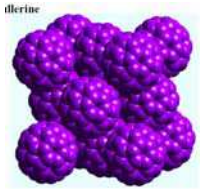
- Atoms are located at each of the corners and on the centers of all the faces of cubic unit cell
- Cu, Al, Ag, Au have this crystal structure



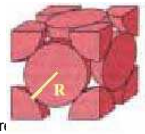


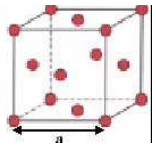
Face-Centered Cubic Crystal Structure (II)

- The hard spheres or ion cores touch one another across a face diagonal ⇒ the cube edge length, **a= 2R√2**
- **The coordination number, CN** = the number of closest neighbors to which an atom is bonded = number of touching atoms, **CN = 12**
- **Number of atoms per unit cell, n = 4**. (For an atom that is shared with m adjacent unit cells, we only count a fraction of the atom, 1/m). In FCC unit cell we have: 6 face atoms shared by two cells: 6 x 1/2 = 3 8 corner atoms shared by eight cells: 8 x 1/8 = 1
- **Atomic packing factor, APF** = fraction of volume occupied by hard spheres = (Sum of atomic volumes)/(Volume of cell) **= 0.74** (maximum possible)



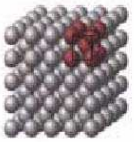
C_{60}

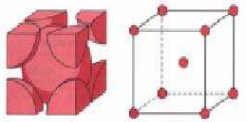


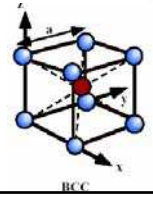


Body-Centered Cubic (BCC) Crystal Structure (I)

- Atom at each corner and at center of cubic unit cell
- Cr, α-Fe, Mo have this crystal structure





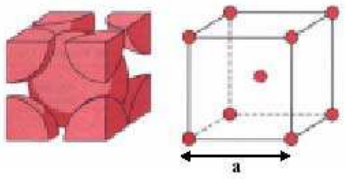


Body-Centered Cubic Crystal Structure (II)

- The hard spheres touch one another along cube diagonal
- ⇒ the cube edge length, **a= 4R/√3**
- **The coordination number, CN = 8**
- **Number of atoms per unit cell, n = 2**
- Center atom (1) shared by no other cells: 1 x 1 = 1
- 8 corner atoms shared by eight cells: 8 x 1/8 = 1

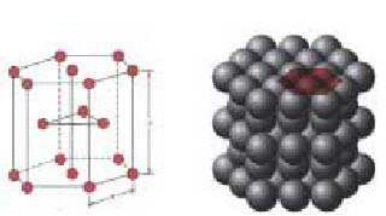
Atomic packing factor, APF = 0.68

- Corner and center atoms are equivalent



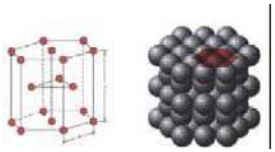
Hexagonal Close-Packed Crystal Structure (I)

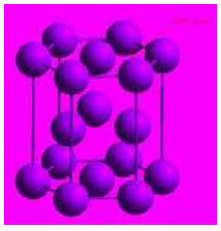
- HCP is one more common structure of metallic crystals
- Six atoms form regular hexagon, surrounding one atom in center. Another plane is situated halfway up unit cell (c-axis), with 3 additional atoms situated at interstices of
- hexagonal (close-packed) planes
- Cd, Mg, Zn, Ti have this crystal structure



Hexagonal Close-Packed Crystal Structure (II)

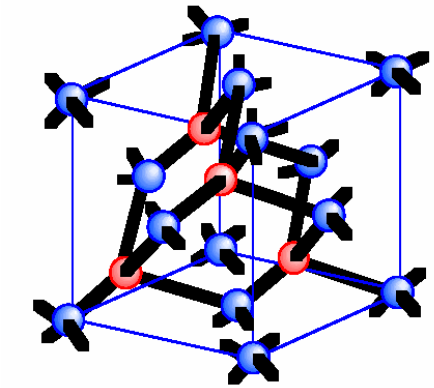
- Unit cell has two lattice parameters a and c. Ideal ratio
- c/a = 1.633
- **The coordination number, CN = 12 (same as in FCC)**
- **Number of atoms per unit cell, n = 6**.
- 3 mid-plane atoms shared by no other cells: 3 x 1 = 3
- 12 hexagonal corner atoms shared by 6 cells: 12 x 1/6 = 2
- 2 top/bottom plane center atoms shared by 2 cells: 2 x 1/2 = 1
- **Atomic packing factor, APF = 0.74 (same as in FCC)**
- All atoms are equivalent





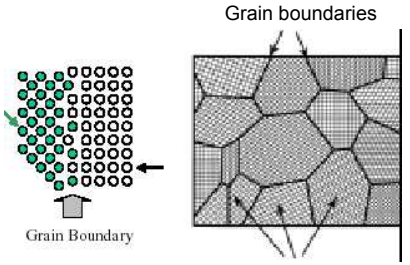
Basic diamond crystal structure

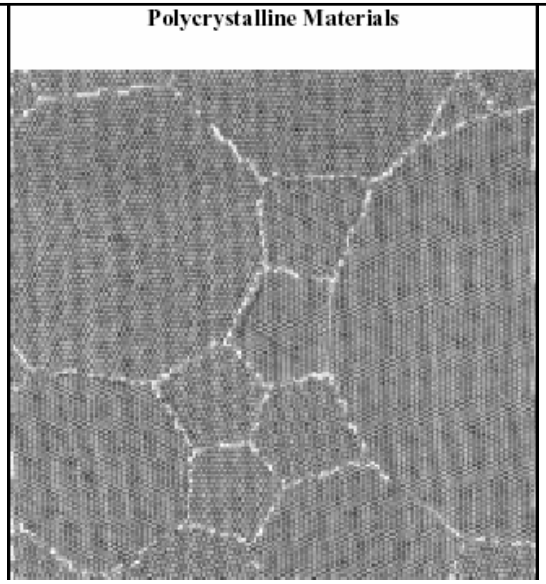
- **Silicon has the basic diamond crystal structure – two merged FCC cells offset by a/4 in x, y and z.**



Single Crystals and Polycrystalline Materials

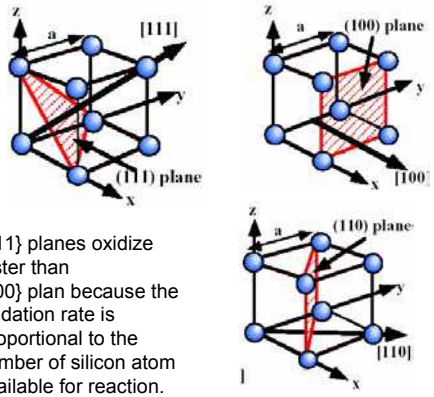
- **Single crystal**: atoms are in a repeating or periodic array
- over the entire extent of the material
- **Polycrystalline material:** comprised of many small
- crystals or **grains.** The grains have different crystallographic orientation.
- There exist atomic mismatch within the regions where grains meet. These regions are called **grain boundaries**.





Crystal Planes and directions

- **Planes and directions are defined using an x, y, z coordinate system.**
- **[111] direction is defined by a vector having components of 1 unit in x, y and z.**
- **Planes are defined by Miller-indices reciprocals of the intercepts of the plane with the x, y and z axes.**



{111} planes oxidize faster than {100} plan because the oxidation rate is Proportional to the number of silicon atom available for reaction.

{111} planes in silicon have a largest number of atom/cm-3 {100} planes the lowest.

Defects in crystal

- **Nothing in Nature is perfect, and crystals are no exception. Any real crystal contains defects, and these affect its properties in various ways.**
- **Defects in diamond alter the colour;**
- **defects in semiconductors (of the right kind) allow them to be used to make devices;**
- **defects in metals alter their mechanical properties;**
- **defects affect thermal and electrical conductivity.**

Beneficial (crystal defects)

- Deep states are added to increase the resistively (> 106 W - cm) of semiconductor material used as substrates (semi-insulating material). The best examples are GaAs:Cr and InP:Fe.
- GaP is an efficient emitter of light. The red light is observed if the crystal contains oxygen together with Zn or Cd. The light is green if GaP is doped with nitrogen and the yellow emission from GaP is obtained by Mg-O doping.
- An increase of switching frequency in silicon junction is obtained by added Gold as deep levels.
- Sensitizing Centers have a large capture cross section for minority carrier , and hence magnitude of photoconductivity, is greatly increased.
- *Thus deep levels are essential for the designing of devices and for their efficient performance.*

Detrimental (crystal defects)

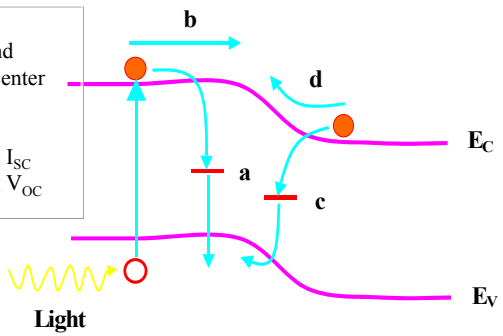
- ❖ Deep level defects may efficiently reduce the minority carrier-life time. This is the main cause of the decrease in the energy conversion efficiency of solar cells.
- ❖ Deep levels may increase the leakage current of devices and also deteriorate the efficiency of photovoltaics.
- ❖ The performance of devices such as light-emitting diodes (LED) is degraded when the deep levels produce a parallel non-radiative recombination path and act as a poison center.
- ❖ Deep level can also act as a Donor or acceptor like , Trap, Killer center and scattering center.
- ➢ Thus reduction of deep levels is essential for the designing of devices and for their efficient performance.

Effects of recombination centers on a solar cell performance

The light-generated minority carrier can return to the ground state through recombination center before being collected by the junction:

i) through path (a) reducing I_{SC}

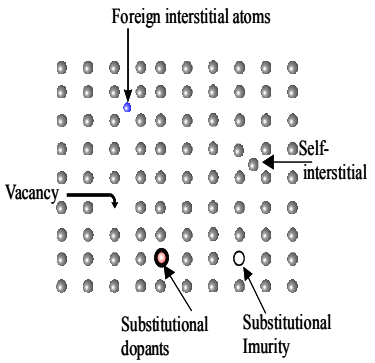
ii) through path (c) reducing V_{OC}



Without recombination centers paths (b) and (d) are dominated

Point defects in semiconductors

- A *point defect* in a crystal is an entity that causes an interruption in the lattice periodicity. This occurs during due to following events:
- An atom is removed from its regular lattice site; the defect is a *vacancy*.
- An atom is in a site different from a regular lattice (substitutional) lattice site; the defect is an *interstitial*. An interstitial defect can be of the same species as the atoms of the lattice (it is an intrinsic defect, the *self-interstitial*) or of a different nature (it is then an extrinsic defect, an interstitial impurity).
- An impurity occupies a substitutional site.

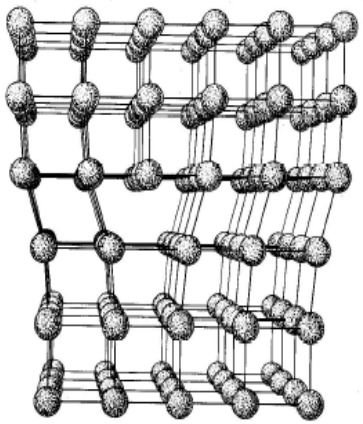


Point defects play critical role in impurity diffusion and in ion implantation as well during space missions.

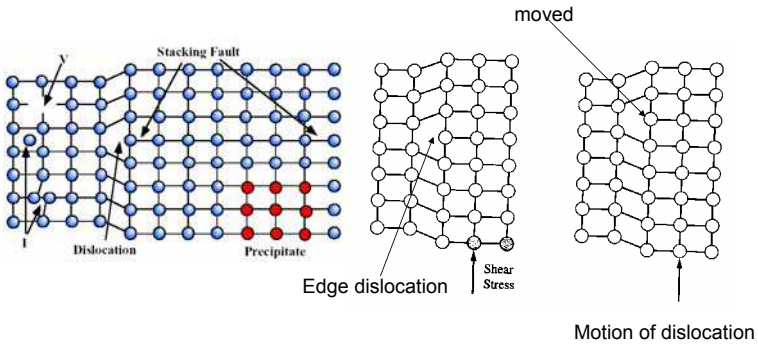
Dislocations

- Dislocations are *line defects*. Simplest to visualize is an *edge dislocation*
- – think of an extra half-plane of atoms.
- Affects deformation properties – to slide upper block over lower now
- only requires a *line* of bonds to break at a time, not a whole *plane* –
- process of *slip*. Explains low yield strength of solids.

- Sources:
  - i by stress due to temperature gradient
  - ii agglomeration

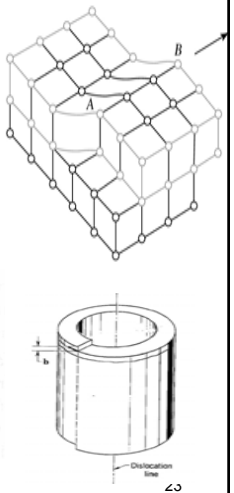


Dislocations move

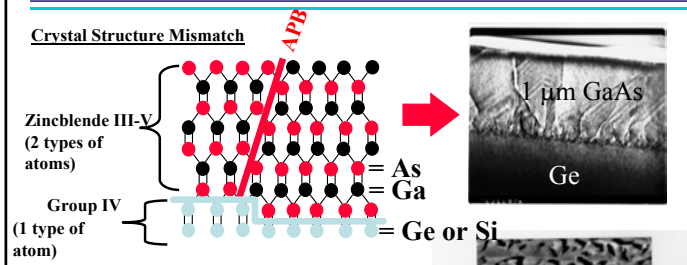


Screw dislocations

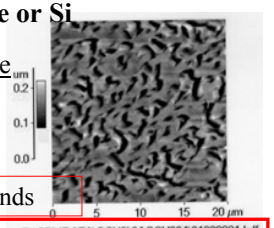
- Screw dislocations give a helical structure to the planes.
- Screw dislocations often show up in crystal growth



Issues: anti-phase domain boundaries (APBs)



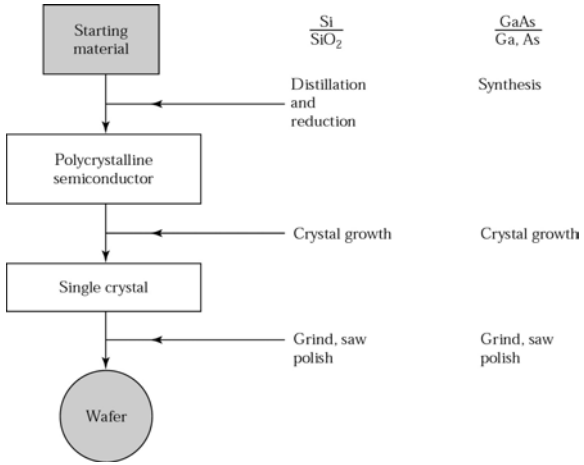
APBs reduce reliability/performance
- Planar shunt/diffusion paths
- surface roughness



Electrically active Ga-Ga or As-As bonds

APD's are a potential problem for <u>any</u> III-V/IV heteroepitaxy!!!

Crystal growth



Process flow from starting material to polished wafer.

Czochralski (CZ) Growth Method

- CZ is more common method to grow silicon crystal today because it is capable of producing large diameter crystals, from which large diameter wafer can be cut.