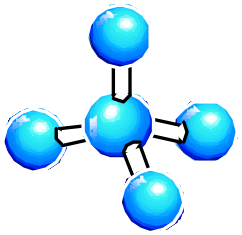
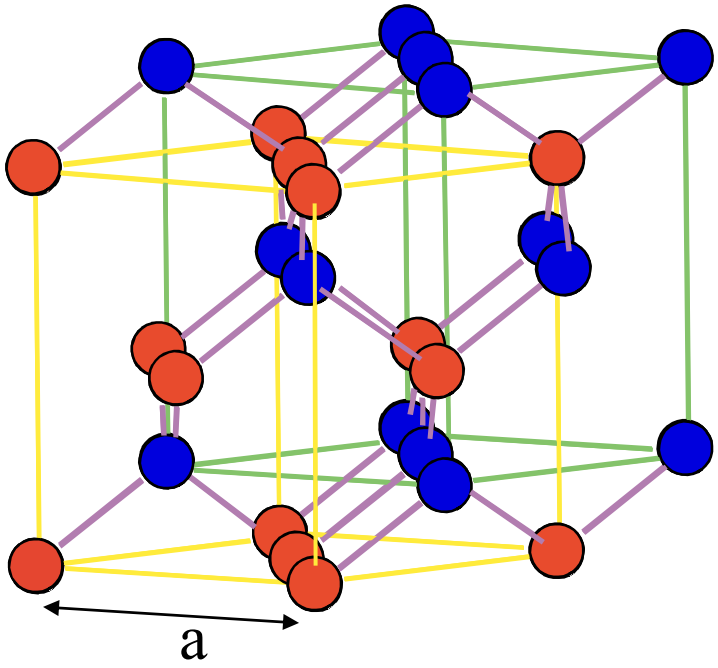
Zincblende crystal structure

- valence 4 structure
  - each atom bonds to four neighbors in a tetragonal configuration



- crystal lattice is face centered cubic (FCC), with two atom basis [at (0,0,0) and (1/4, 1/4, 1/4)]
    - two "interpenetrating" FCC lattices
  - lattice constant "a": cube side length
    - silicon (rm temp): 5.43 Å ; GaAs: 5.65 Å
    - nearest neighbor distance $d_n = \frac{\sqrt{3}}{4} a$
  - atomic density:
    - 4 atoms inside cube
    - 6 atoms "half" inside at face centers
    - 8 atoms 1/8 inside at corners
    - total of 8 atoms per cube: atomic density $8 / a^3$



$\rho_{Si} = 5 \times 10^{22}$ atoms/cm^3

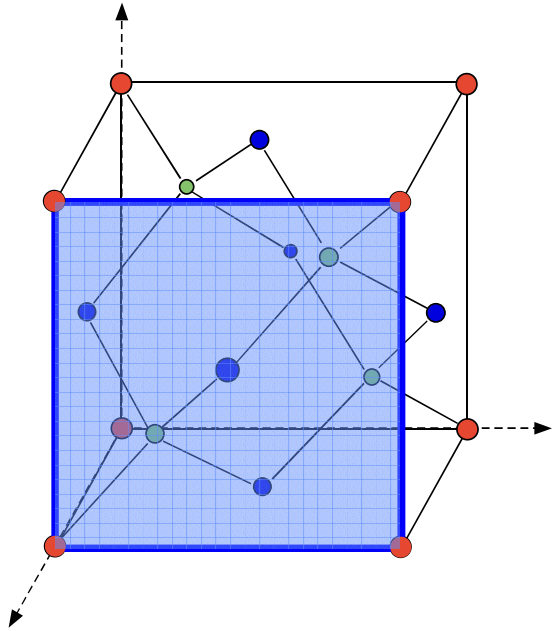
Miller Indices in Crystals

- For a plane with:
  - x-axis intercept x_o
  - y-axis intercept y_o
  - z-axis intercept z_o
  - the Miller indices (hkl) for this plane are given by finding the inverses of x_o, y_o, & z_o and reducing them to the smallest set of integers h: k: l having the same ratio $(x_o)^{-1}$: $(y_o)^{-1}$: $(z_o)^{-1}$.

- Conventions:
  - (hkl): single plane or set of all parallel planes.
  - ($\bar{h}$ kl): for a plane that intercepts the x axis on the negative side of the origin.
  - {hkl}: for all planes of equivalent symmetry, such as {100} for (100), (010), (001), ($\bar{1}$00), (0$\bar{1}$0), and (00$\bar{1}$) in cubic symmetry.
  - [hkl]: for the direction perpendicular to the (hkl) plane.
  - <hkl>: for a full set of equivalent directions.

Low Index Directions In Silicon (Cubic, Diamond Structure)

- (100)



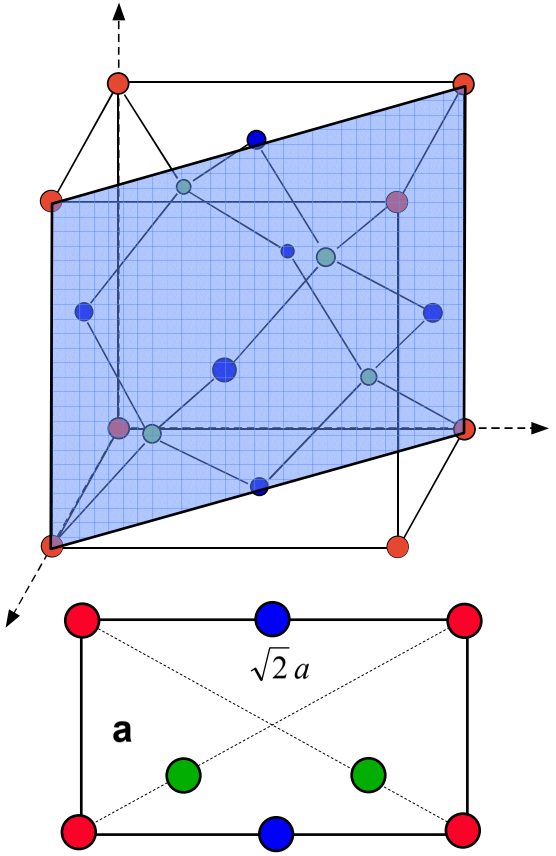
surface atomic density

$$\rho_{100}^{surface} = \frac{(1atom + 4 \cdot [1/4 atom])}{a^2}$$

silicon:

ρ_{100} = 6.8 x 10^{14} atoms / cm^2

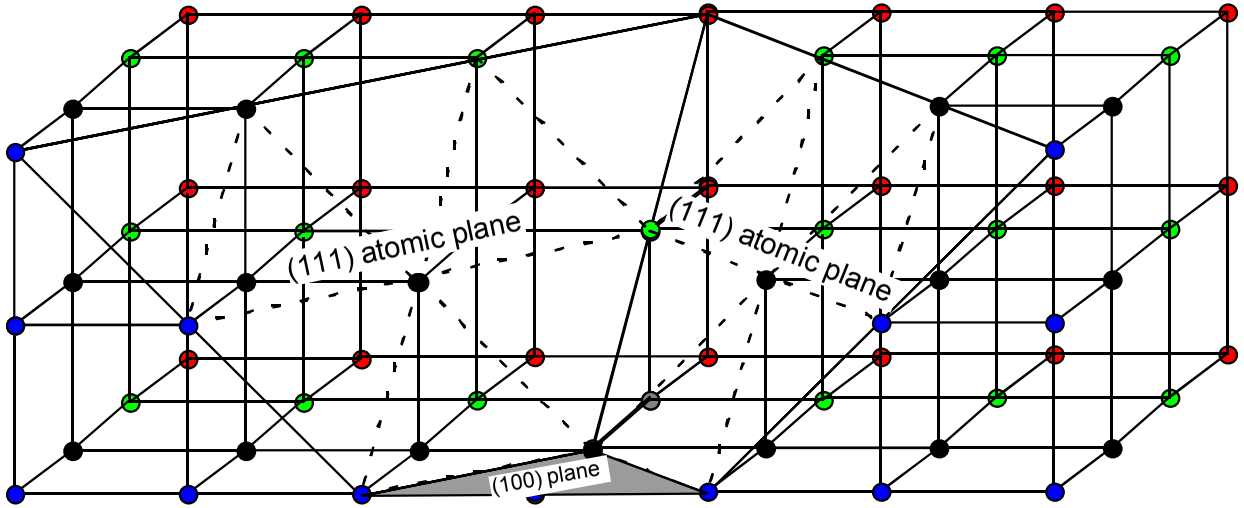
- (110)

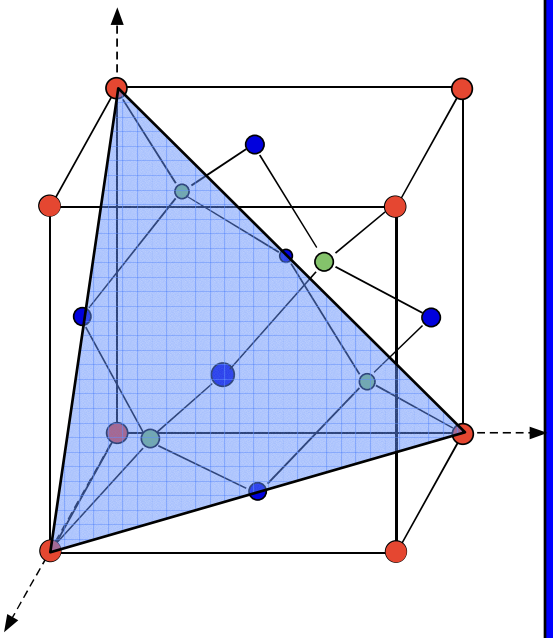


$$\rho_{110}^{surface} = \frac{(2\,\text{atoms} + 4 \cdot [1/4\ \text{atom}] + 2 \cdot [1/2\ \text{atom}])}{\sqrt{2}\,a \cdot a}$$

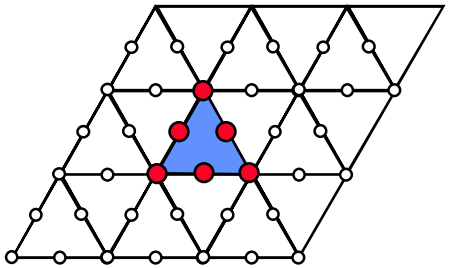
(111) planes

- (111) planes etch the slowest, tend to be cleavage planes





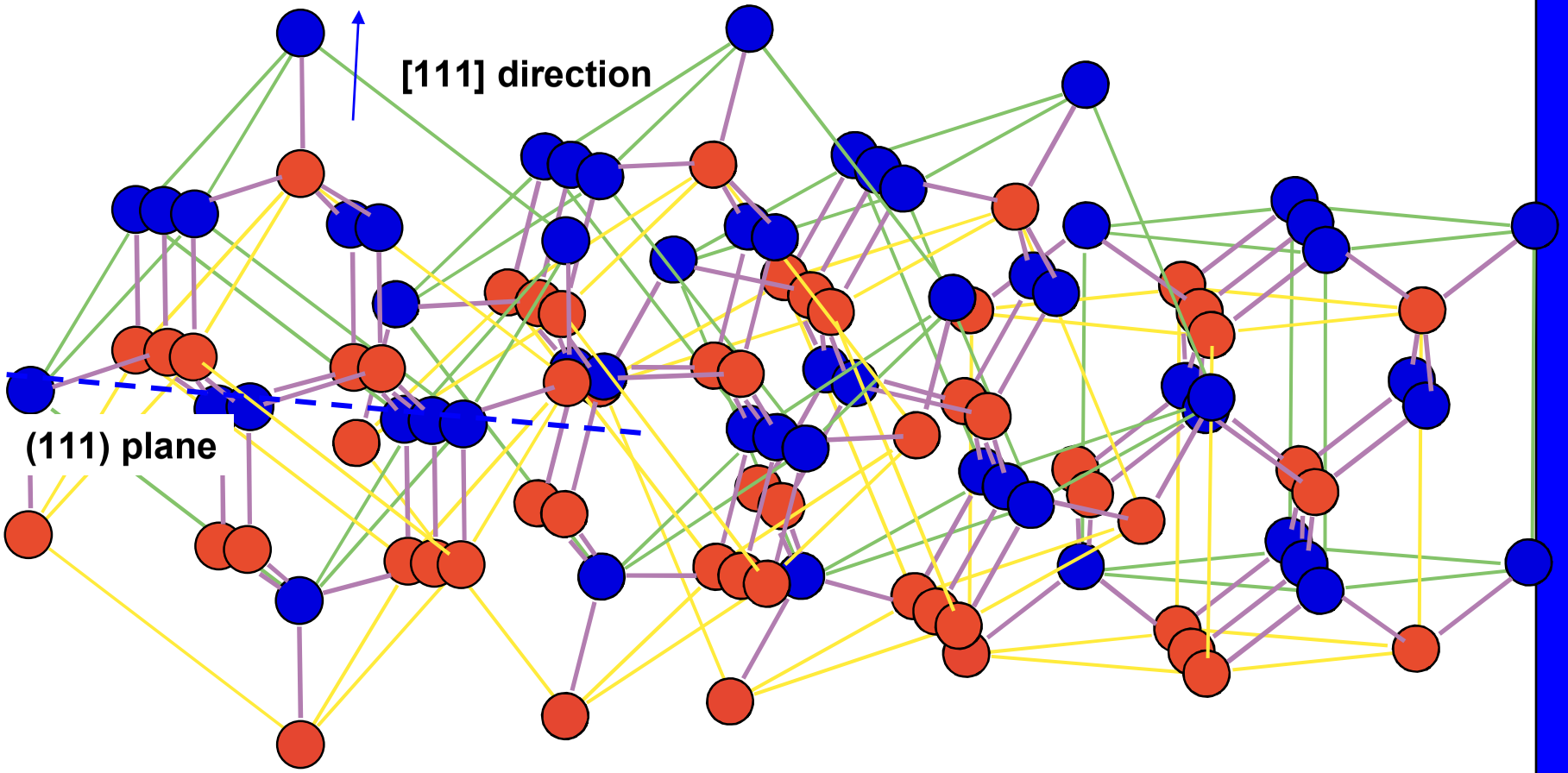
$$\rho_{111}^{surface} = \frac{\left(3 \cdot [1/2 \text{ atom}] + 3 \cdot [1/6 \text{ atom}]\right)}{\sqrt{3}/2 \cdot a^2}$$



- **silicon:**
  7.8 x 10^{14} atoms / cm^2
- **surface atomic density somewhat higher than (100)**

(111) orientation in silicon

- [111] is the “natural” orientation for zincblende crystals



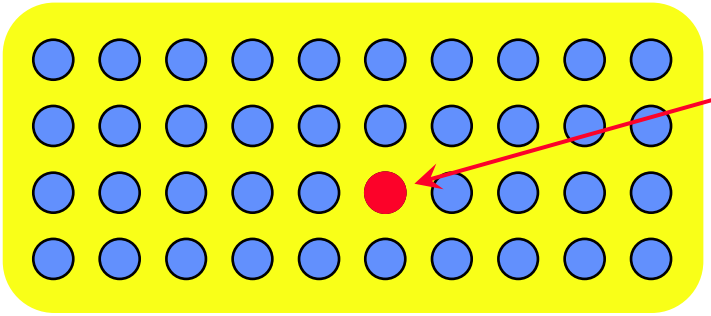
Dopants and impurities in semiconductors

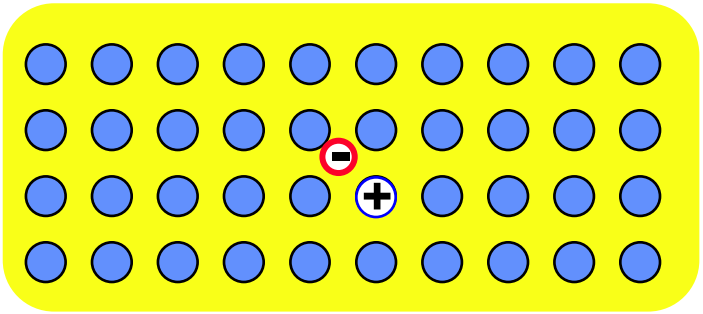
												III	IV	V			
1	1 H																2 He
2	3 Li	4 Be										5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg										13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca		21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr		39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Uun	111 Uuu	112 Uub	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

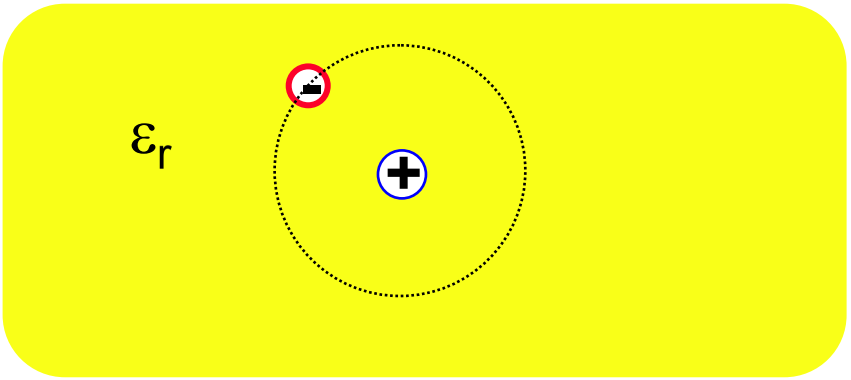
- **For column IV elements (e.g., silicon)**
  - **valence III: one electron "short", acceptor**
    - **boron, aluminum, gallium**
  - **valence V: one "extra" electron, donor**
    - **nitrogen, phosphorus, arsenic, antimony**

Impurity Levels in Semiconductors

- replace impurity with perfect crystal, but with extra fixed charge in the lattice, and free complimentary carrier
- replace crystal with dielectric, replace charges with “hydrogen atom”







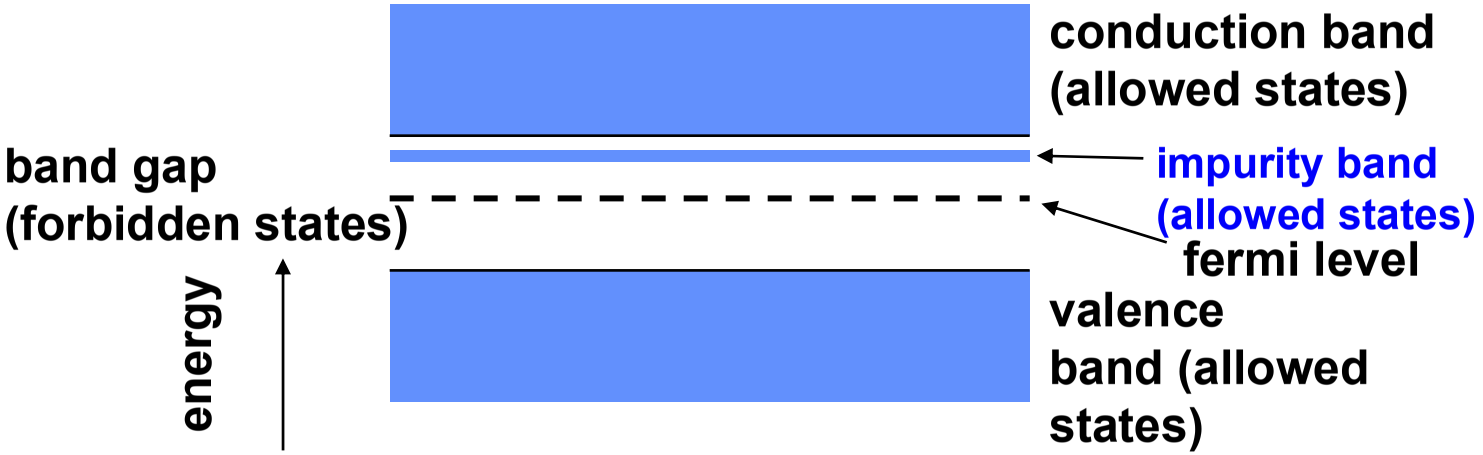
Impurity Levels in Semiconductors

- fixed charge in the lattice and free complimentary carrier introduces a new energy state within the band-gap
- impurity level (for a donor) is superposition of conduction band wavefunctions
  - use hydrogen atom model to calculate the new state location

$$E = -\frac{m\,q^4}{8a^2\,h^2\,(\varepsilon_r\,\varepsilon_o)^2} = -\frac{13.6}{(\varepsilon_r)^2}\,\frac{m^*}{m_{electron}}\,eV$$

    - use static dielectric constant of semiconductor
    - use effective mass from conduction band states
    - net reduction of $\varepsilon_r^2 / (m^* / m_0) \approx 200$
  - $\rightarrow E_d \approx 0.05$ eV

Band diagrams for semiconductors



- Fermi level indicates how states are actually occupied
  - a flat fermi level indicates that no external voltages are applied
  - most above the Fermi level are empty of electrons
  - most below are full of electrons
    - donor levels are empty when "active"
    - acceptor levels are occupied when "active"

Occupancy of impurity levels

- whether state is empty or filled depends on fermi level position and temperature
  - from statistical mechanics, for system with N_j electrons in state j at energy E_j, the occupancy is:

$$\langle n \rangle = \frac{\sum_{\text{states}} N_j \, e^{-(E_j - \mu N_j)/kT}}{\sum_{\text{states}} e^{-(E_j - \mu N_j)/kT}}$$

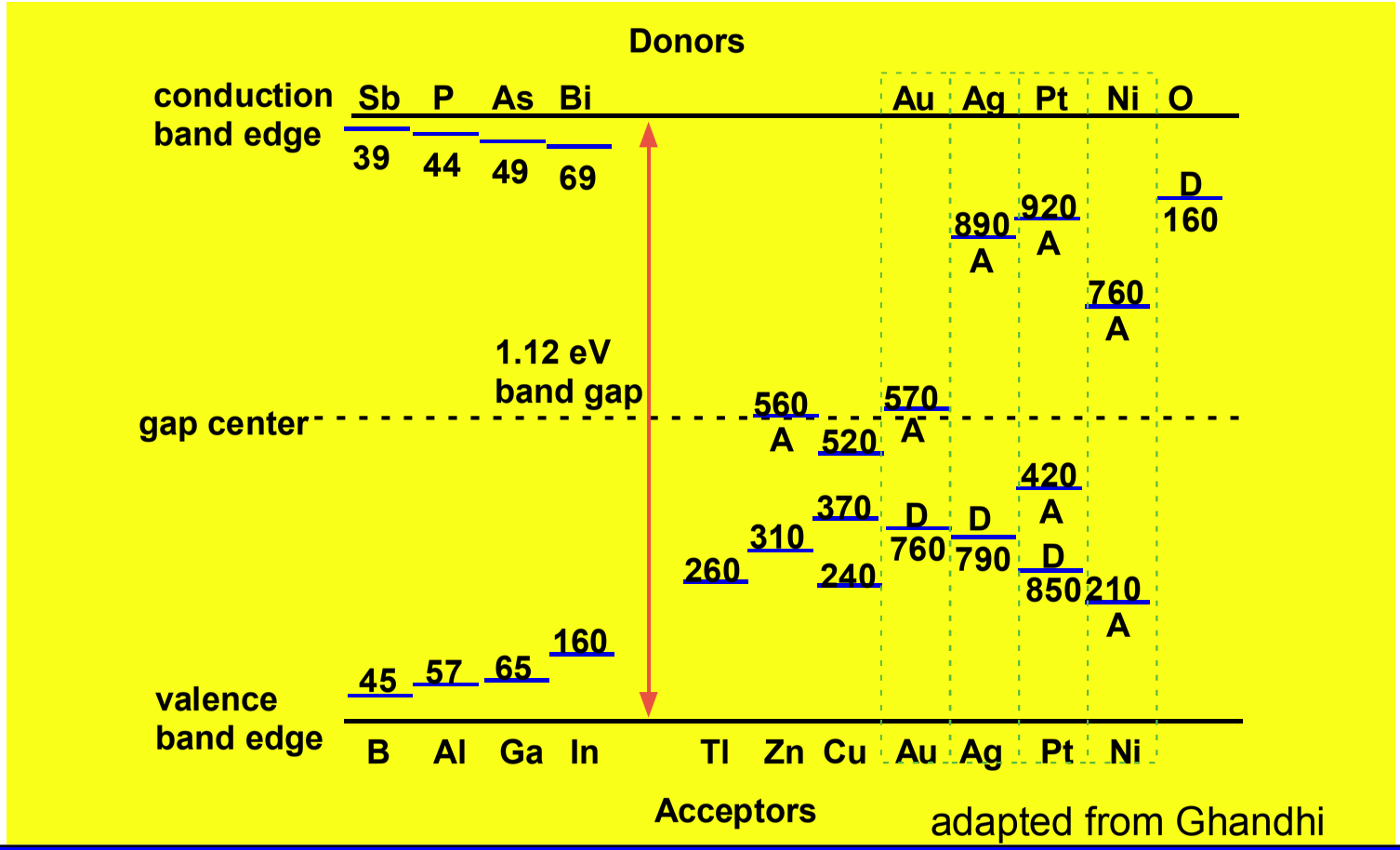
  - for a donor we have three states
    - no electrons in state: $N_j = 0$, $E_j = 0$
    - one spin up electron in state: $N_j = 1$, $E_j = E_{imp}$
    - one spin down electron: $N_j = 1$, $E_j = E_{imp}$

$$\langle n \rangle = \frac{2e^{-(E_{imp} - \mu)/kT}}{1 + 2e^{-(E_{imp} - \mu)/kT}} = \frac{1}{1 + \frac{1}{2} e^{(E_{imp} - \mu)/kT}}$$

  - for complete ionization (all donors "active") need occupancy = 0
    - must have $E_{imp} - \mu >> kT$!!
    - impurity level must be several kT above the fermi level!

Impurities in silicon

- impurity levels in meV from band edge
  - A: acceptor-like behavior
  - D: donor-like behavior



Impurities in Silicon

- **Oxygen: (column VI)**
  - **common unintentional impurity from silica crucibles**
    - **10^{16} - 10^{18} cm^{-3}**
    - **usually clumps with silicon into large (~1μm) SiO_2 complexes; sensitive to processing history**
- **Carbon: (column IV)**
    - **high solid solubility ($4x10^{18}$)**
    - **mainly substitutional, electrically inactive**
- **Gold:**
    - **deep donor or acceptor**
    - **rapid diffuser**
    - **minority carrier lifetime "killer"**

Impurities in GaAs

- Zinc: (column II)
  - very common p-type dopant
  - substitutional on Ga site to 10^{21}
- Sulfur: (column VI)
  - very common n-type dopant
  - substitutional on As sites to 10^{18}
- Silicon: (column IV)
  - common unintentional contaminant
  - amphoteric; site selection depends on temperature history (As or Ga vacancy concentrations)
- Chromium and Iron:
  - deep level impurities
  - chromium intentionally introduced (10^{17}) to form semi-insulating (10^{9} Ω cm) GaAs
- Almost all GaAs is compensated, i.e. contains both ionized donors and acceptors:
  - $n \cong N_D - N_A$
  - compensation ratio = $(N_D + N_A)/n$

Tetrahedral radii and misfit factors

- calculated radii in “diamond” lattice
- misfit relative to silicon radius

element r_{tet} Si misfit %		B 0.88Å -25%	C 0.77Å	N 0.70Å	O 0.66Å
		Al 1.26Å	Si 1.17Å	P 1.10Å -6.8%	S 0.99Å
Cu 1.35Å	Zn 1.31Å	Ga 1.26Å +6.8%	Ge 1.22Å	As 1.18Å 0%	Se 1.14Å
Ag 1.52Å	Cd 1.48Å	In 1.44Å	Sn 1.40Å	Sb 1.36Å +15%	Te 1.32Å
Au +27%	Hg 1.48Å	Tl	Pb	Bi	Po

Solid solubility limits in Si

- solid solubility: maximum equilibrium concentration of impurity (solute) in host material (solvent)
  - temperature dependent
  - generally lower at lower temp
  - @ 1000˚C

element
$N_{solid\ sol}$ (cm^{-3})

		B 1.5×10^{20}	C	N
		Al 2×10^{19}	Si	P 10^{21}
Cu	Zn	Ga 3×10^{19}	Ge	As 2×10^{21}
Ag	Cd	In	Sn	Sb 4×10^{19}
Au 10^{16}	Hg	Tl	Pb	Bi

Defects in crystals

- point defects
  - "zero" dimensional
  - most common, lowest energy of formation
- dislocations or line defects
  - one dimensional
  - collection of continuous point defects
- area (planar) defects
  - two dimensional
  - gross change in crystal "orientation" across a surface

Point Defects in Crystals

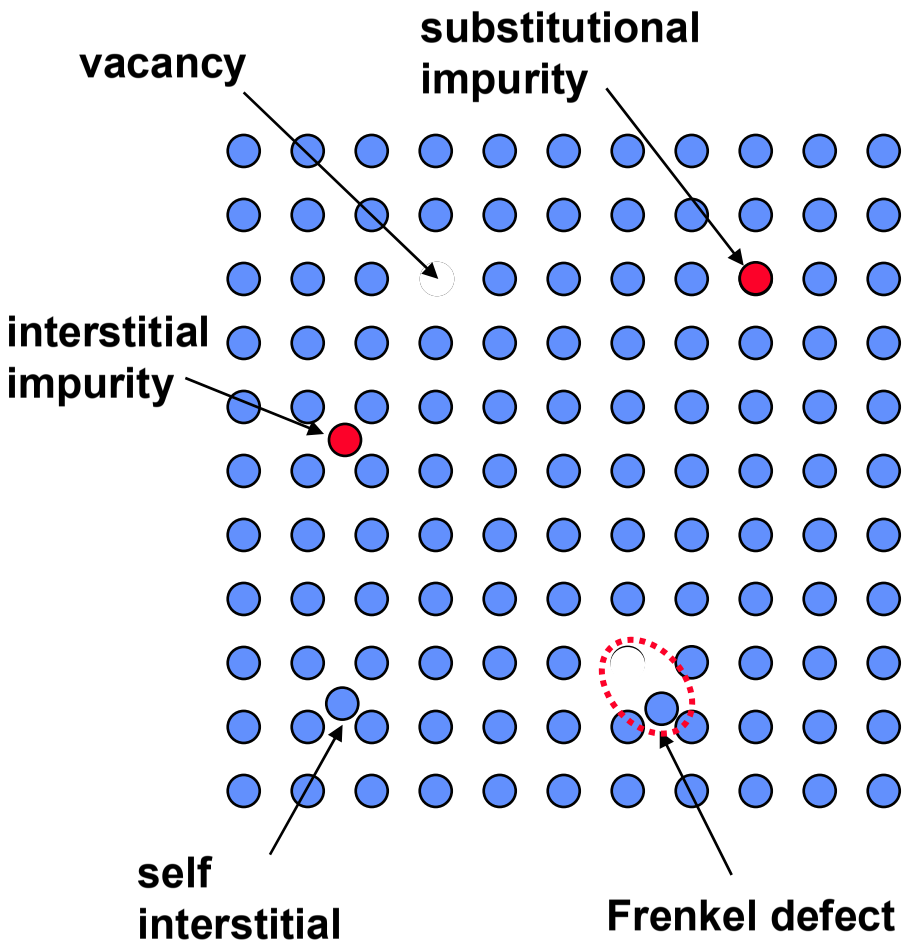
- vacancy , interstitial , substitutional
  - isolated vacancy: Schottky defect

$$n \cong N_{atomic}\, e^{-E/kT}$$

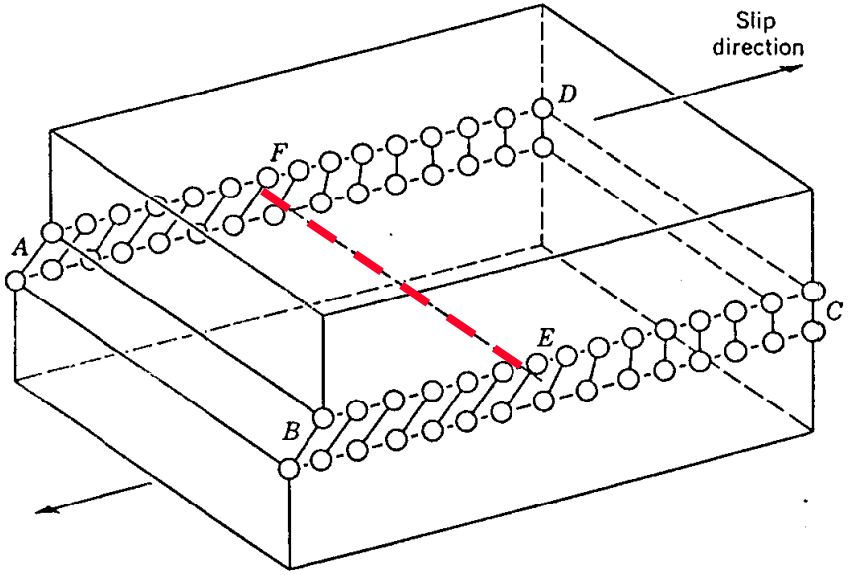
    - $E_{formation}$ ~ 2 eV
      - T = 300K: n ~ 0
      - T = 1300K: $n \sim 10^{13}$
  - vacancy-interstitial pair: Frenkel defect

$$n \cong N_{atomic}\, e^{-E/2kT}$$

    - $E_{formation}$ ~ 1 eV
      - T = 300K: $n \sim 10^{13}$
      - T = 1300K: $n \sim 10^{20}$

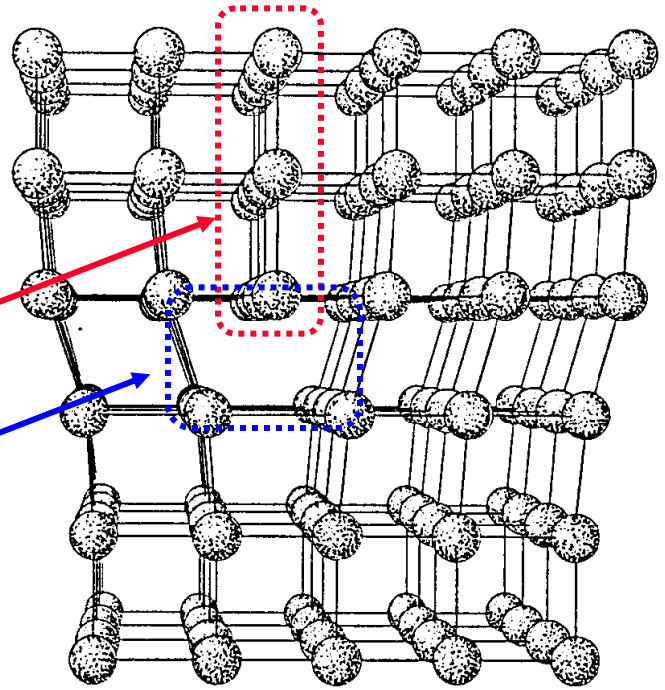


Edge Dislocations



$\overline{EF}$ is dislocation line

- one dimensional defect
  - formation energy is high, concentration usually low

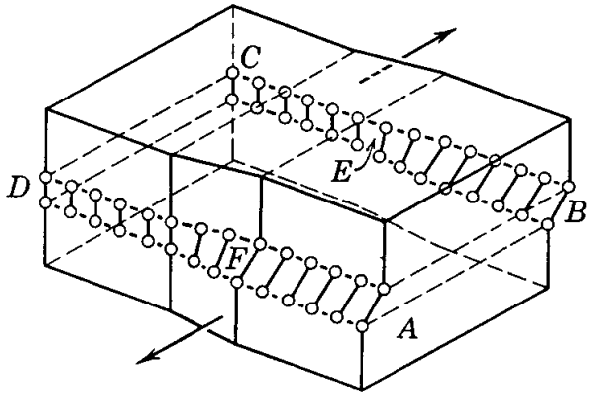


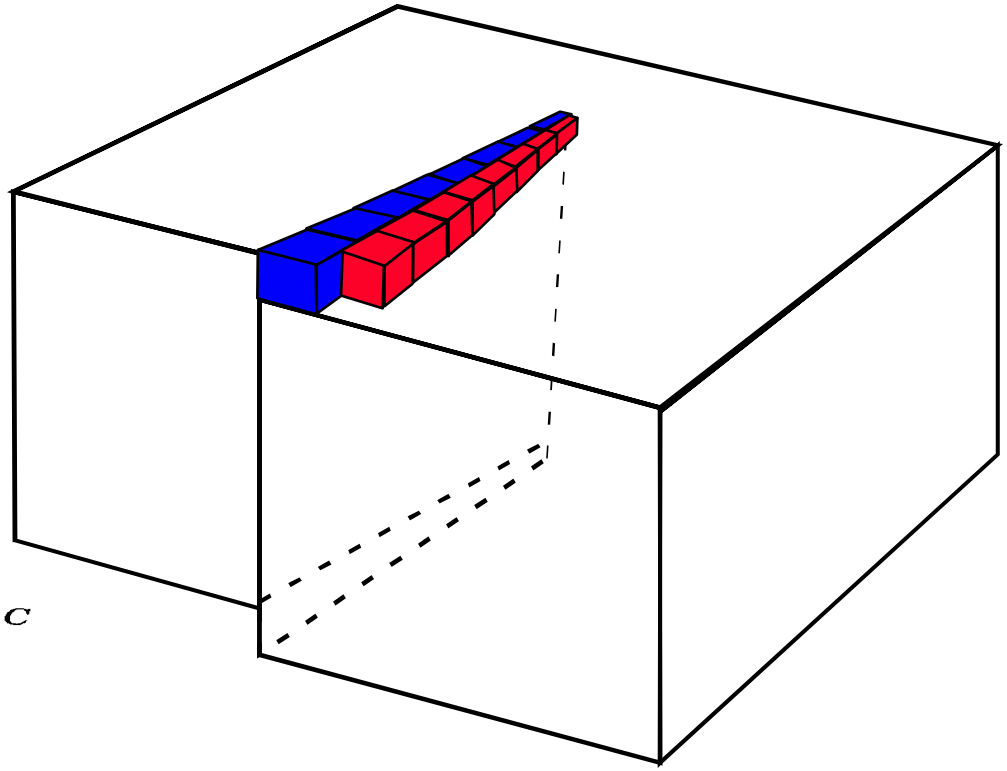
"extra" plane of atoms

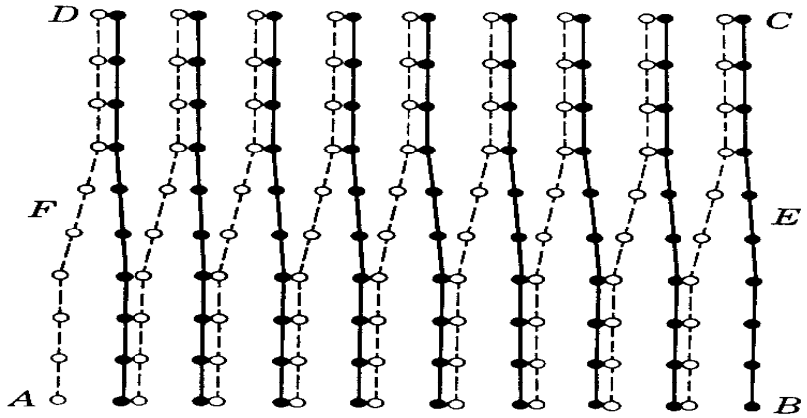
dislocation

from Kittel, p. 591

Screw Dislocation (1-d defect)







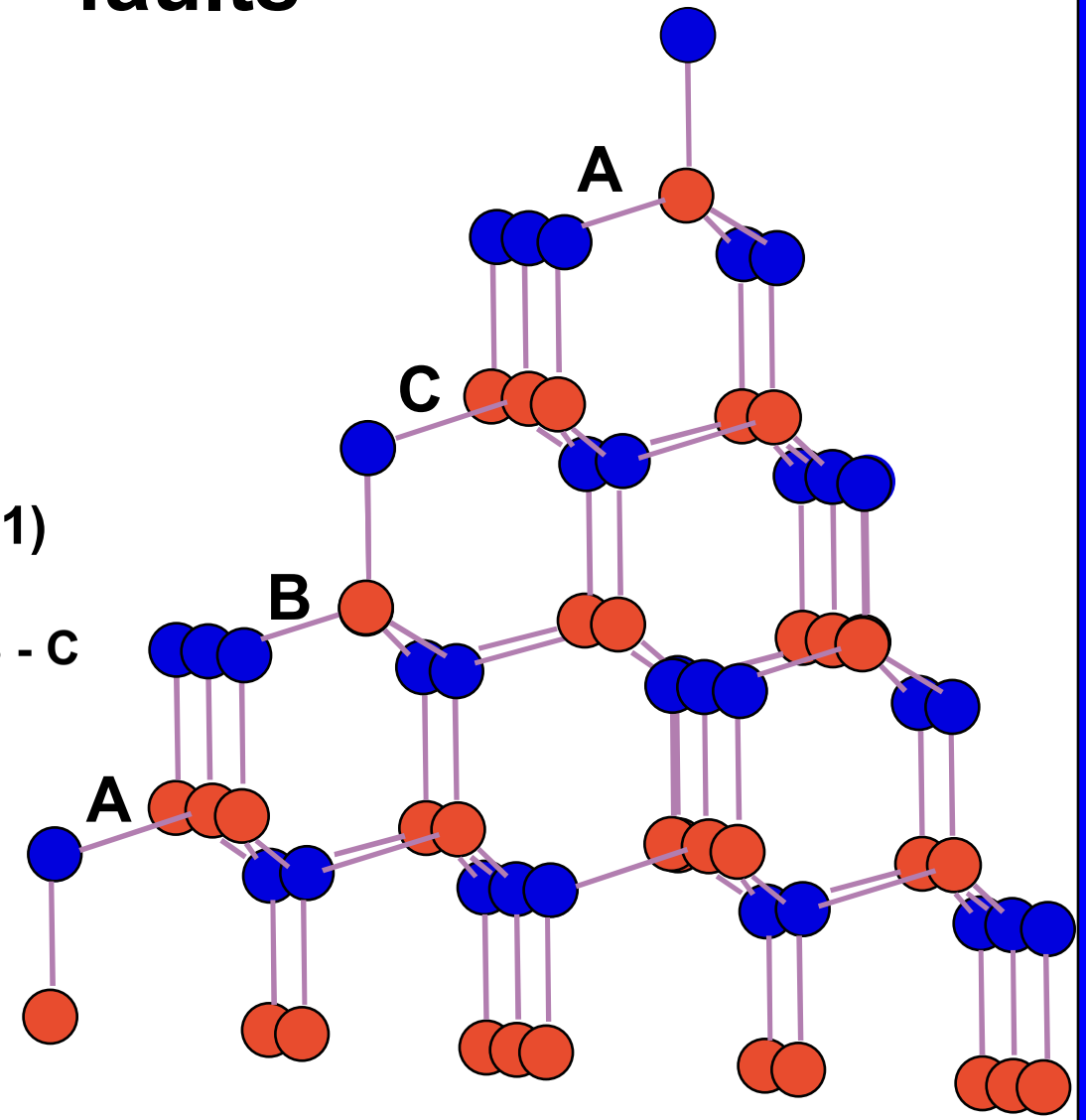
- **screw dislocations are most commonly formed during crystal growth**

Stacking arrangement and stacking faults

- layer ordering:

  A B C A B C

- planar (2-d) defect
  - stacking fault: missing or extra (111) plane
    - A - B - C - C - A - B - C
    - A - B - A - B - C



Bulk crystal growth