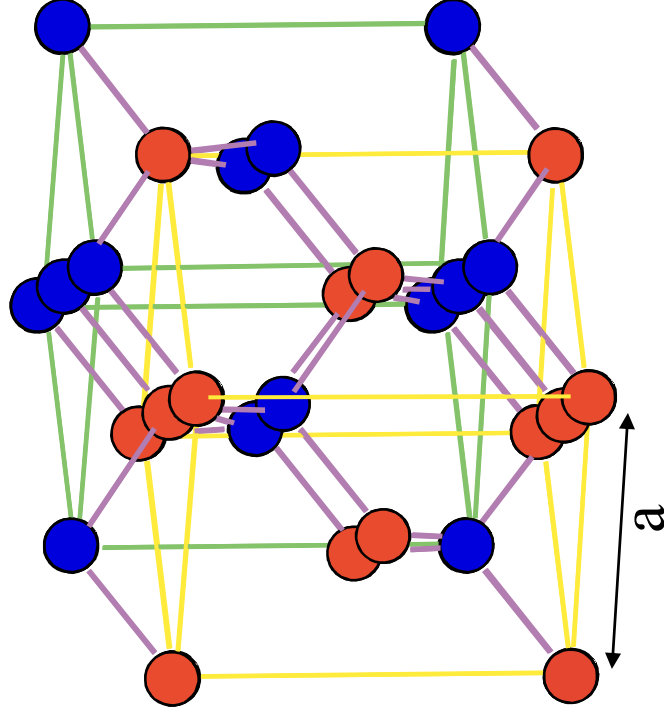
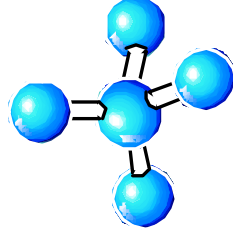


Zincblende crystal structure

- 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 $8 / a^3$



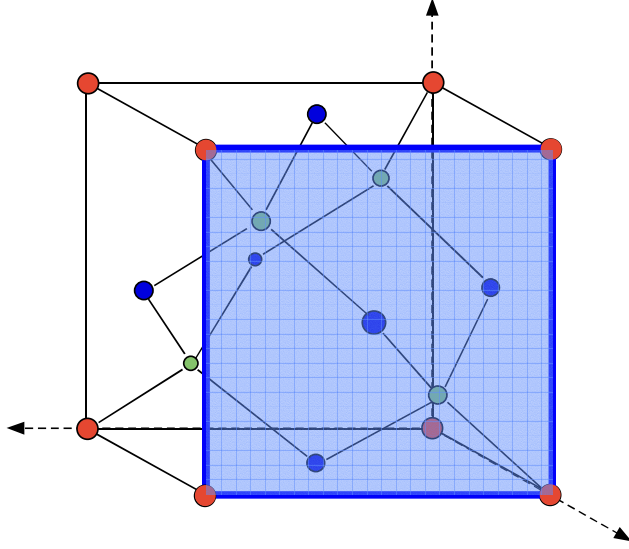
$$\rho_{\text{Si}} = 5 \times 10^{22} \text{ atoms/cm}^3$$

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)



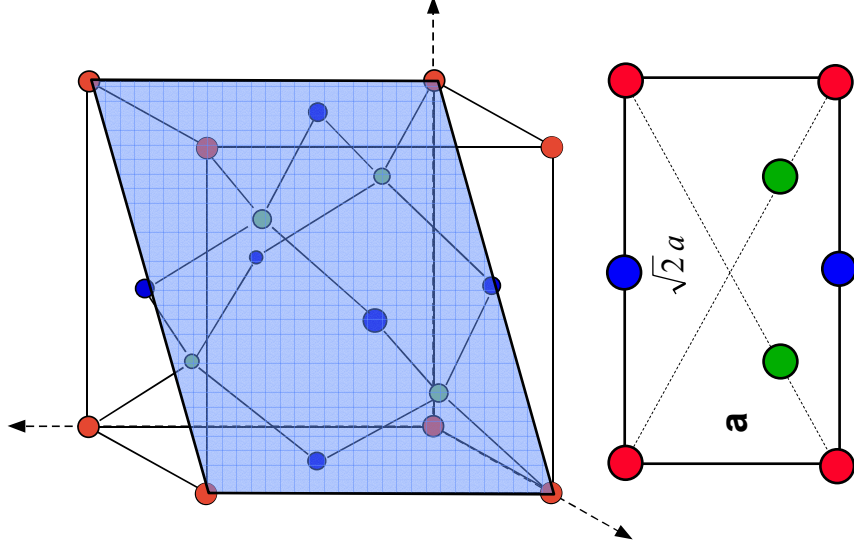
surface atomic density

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

silicon:

$$\rho_{100} = 6.8 \times 10^{14} \text{ atoms / cm}^2$$

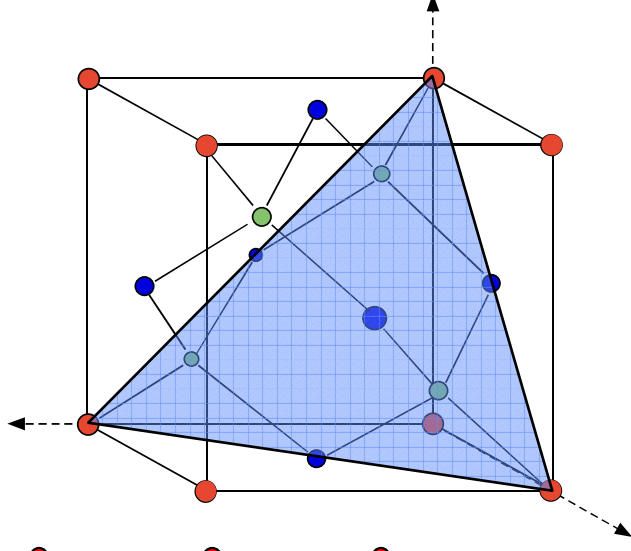
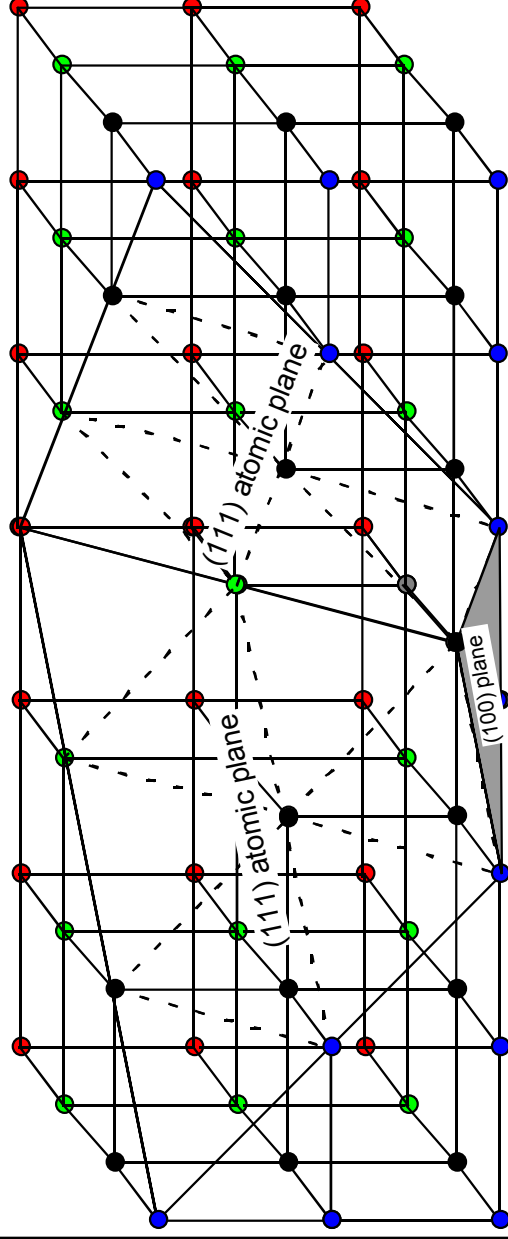
• (110)



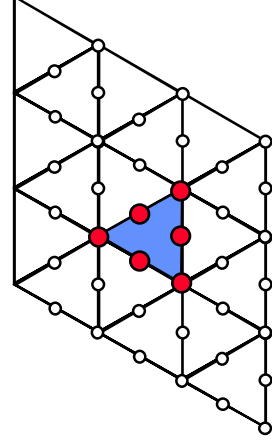
$$\rho_{110}^{surface} = \frac{(2atoms + 4 \cdot [\frac{1}{4} atom] + 2 \cdot [\frac{1}{2} atom])}{\sqrt{2} a \cdot a}$$

(111) planes

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



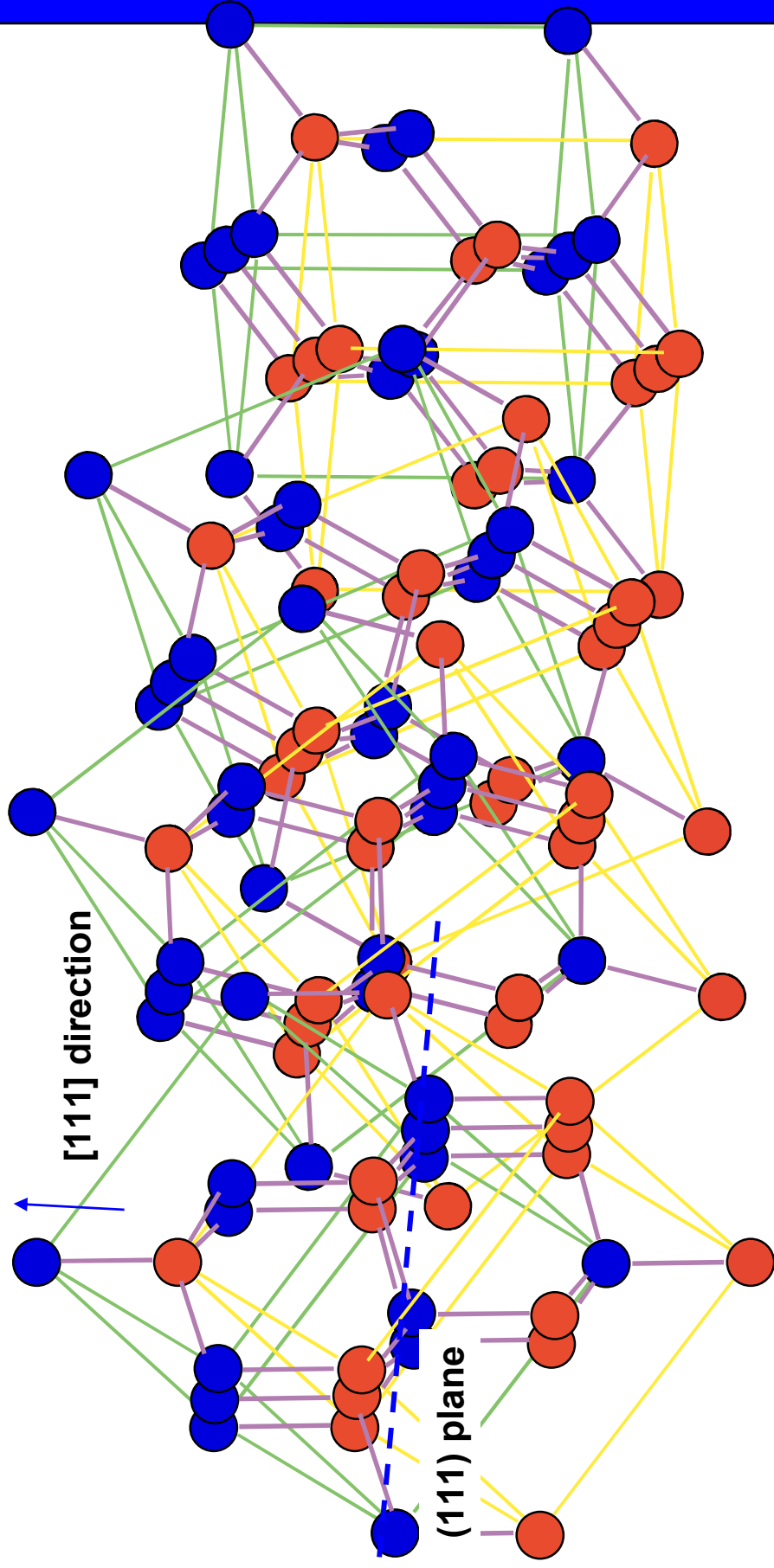
$$\rho_{111}^{\text{surface}} = \frac{3 \cdot \left[\frac{1}{2} \text{atom} \right] + 3 \cdot \left[\frac{1}{6} \text{atom} \right]}{\sqrt{3}/2 \cdot a^2}$$



- silicon:
7.8 x 10¹⁴ atoms / cm²
- surface atomic density somewhat higher than (100)

(111) orientation in silicon

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



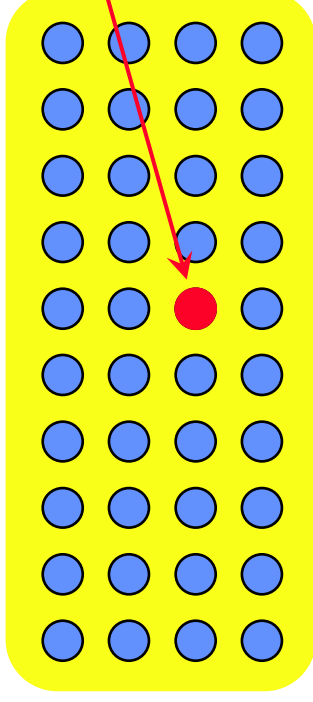
Dopants and impurities in semiconductors

Author: [Mark Winter](#) [[WebElements Ltd](#) and [University of Sheffield](#), England]
 WebElements™, the periodic table on the WWW,
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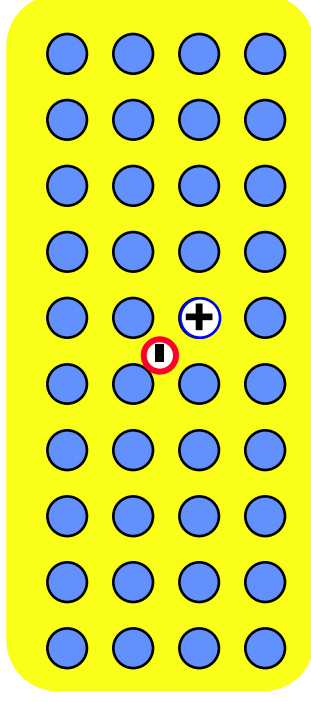
1	<u>H</u>	2	<u>He</u>
3	<u>Li</u>	9	<u>F</u>
4	<u>Be</u>	17	<u>Cl</u>
11	<u>Na</u>	18	<u>Ar</u>
12	<u>Mg</u>	36	<u>Kr</u>
20	<u>Ca</u>	54	<u>Xe</u>
37	<u>Rb</u>	86	<u>Rn</u>
55	<u>Cs</u>	111	<u>Uu</u>
87	<u>Fr</u>	118	<u>Og</u>
21	<u>Sc</u>	39	<u>Y</u>
22	<u>Ti</u>	40	<u>Zr</u>
23	<u>V</u>	41	<u>Nb</u>
24	<u>Cr</u>	42	<u>Mo</u>
25	<u>Mn</u>	43	<u>Tc</u>
26	<u>Fe</u>	44	<u>Ru</u>
27	<u>Co</u>	45	<u>Rh</u>
28	<u>Ni</u>	46	<u>Pd</u>
29	<u>Cu</u>	47	<u>Ag</u>
30	<u>Zn</u>	48	<u>Cd</u>
31	<u>Ga</u>	49	<u>In</u>
32	<u>Ge</u>	50	<u>Sn</u>
33	<u>As</u>	51	<u>Sb</u>
34	<u>Se</u>	52	<u>Te</u>
35	<u>Br</u>	53	<u>I</u>
36	<u>Kr</u>	54	<u>Xe</u>
51	<u>Sb</u>	83	<u>Bi</u>
52	<u>Te</u>	84	<u>Po</u>
53	<u>I</u>	85	<u>At</u>
54	<u>Xe</u>	86	<u>Rn</u>
81	<u>Tl</u>	82	<u>Pb</u>
82	<u>Pb</u>	83	<u>Bi</u>
83	<u>Bi</u>	84	<u>Po</u>
84	<u>Po</u>	85	<u>At</u>
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Impurity Levels in Semiconductors

- replace impurity with perfect crystal, but with extra fixed charge in the lattice, and free complimentary carrier

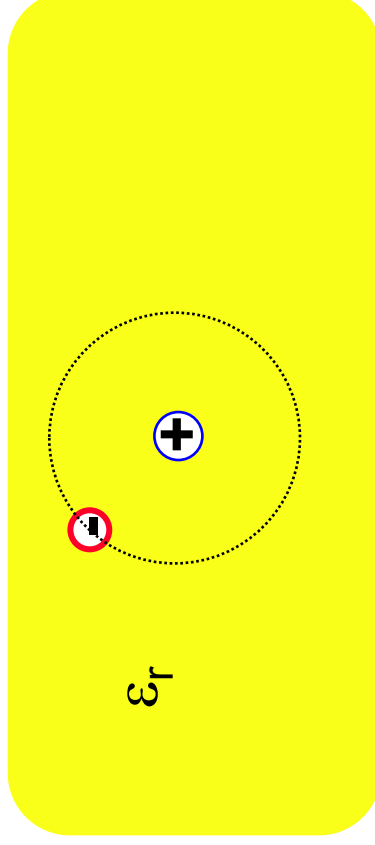


donor in
crystal



fixed charge /
"bound"
electron"

- replace crystal with dielectric, replace charges with "hydrogen atom"



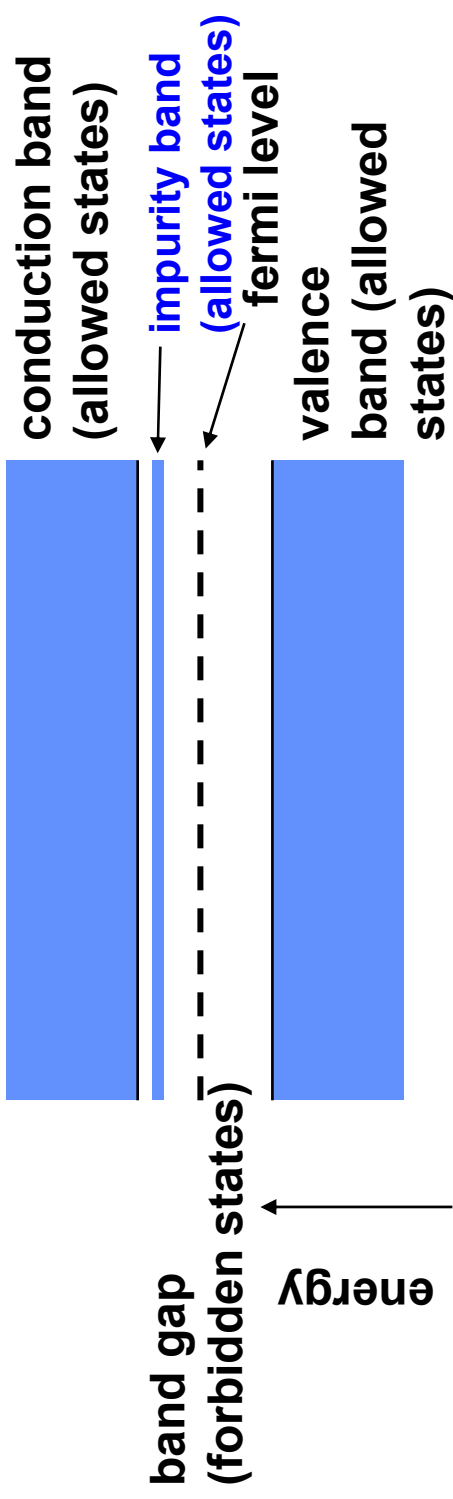
Impurity Levels in Semiconductors

- 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

$$E = -\frac{m q^4}{8 a^2 h^2 (\epsilon_r \epsilon_0)^2} = -\frac{13.6}{(\epsilon_r)^2} \frac{m^*}{m_{\text{electron}}} \text{eV}$$

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

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

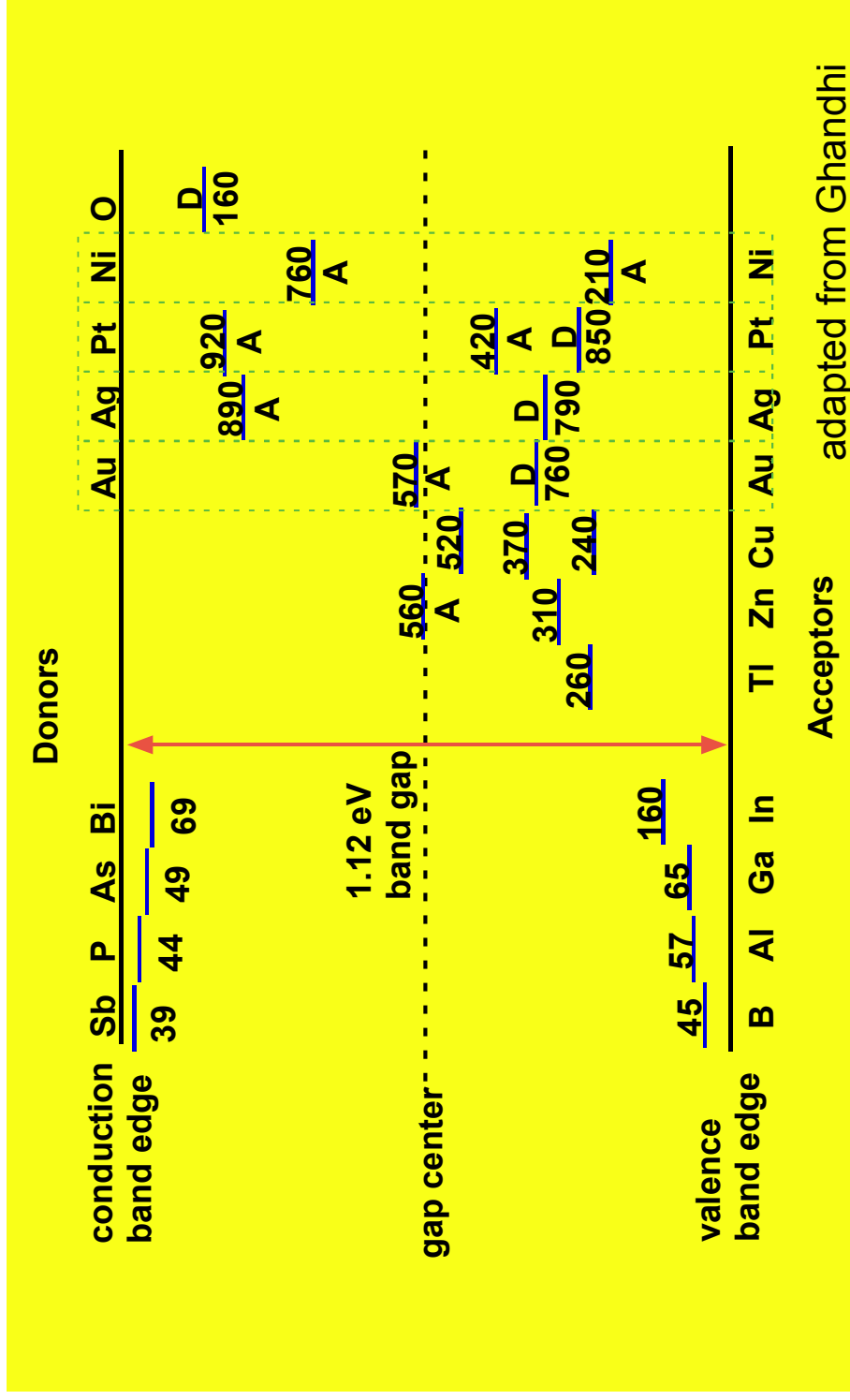
- whether state is empty or filled depends on fermi level position and temperature
 - from statistical mechanics, for system with N_j electrons in state j at energy E_j , the occupancy is:
$$\langle n \rangle = \frac{\sum_{\text{states}} N_j e^{-(E_j - \mu N_j) / kT}}{\sum_{\text{states}} e^{-(E_j - \mu N_j) / kT}}$$
 - for a donor we have three states
 - no electrons in state: $N_j = 0, E_j = 0$
 - one spin up electron in state: $N_j = 1, E_j = E_{\text{imp}}$
 - one spin down electron: $N_j = 1, E_j = E_{\text{imp}}$

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

- for complete ionization (all donors “active”) need occupancy = 0
 - must have $E_{\text{imp}} - \mu \gg kT$!!
 - **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
 - $10^{16} - 10^{18} \text{ cm}^{-3}$
 - usually clumps with silicon into large ($\sim 1\mu\text{m}$) SiO_2 complexes; sensitive to processing history
- **Carbon: (column IV)**
 - high solid solubility (4×10^{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 ($10^9 \Omega \text{ cm}$) 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	B	C	N	O
r_{tet}	0.88Å -25%	0.77Å	0.70Å	0.66Å
Si misfit %	Al 1.26Å	Si 1.17Å	P 1.10Å -6.8%	S 0.99Å
Cu 1.35Å	Ga 1.26Å +6.8%	Ge 1.22Å	As 1.18Å 0%	Se 1.14Å
Ag 1.52Å	In 1.44Å	Sn 1.40Å	Sb 1.36Å +15%	Te 1.32Å
Au +27%	Tl 1.48Å	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	$N_{\text{solid sol}}$ (cm^{-3})	
Cu	Zn	
Ag	Cd	
Au 10^{16}	Hg	
B 1.5×10^{20}	C	N
Al 2×10^{19}	Si	P 10^{21}
Ga 3×10^{19}	Ge	As 2×10^{21}
In	Sn	Sb 4×10^{19}
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

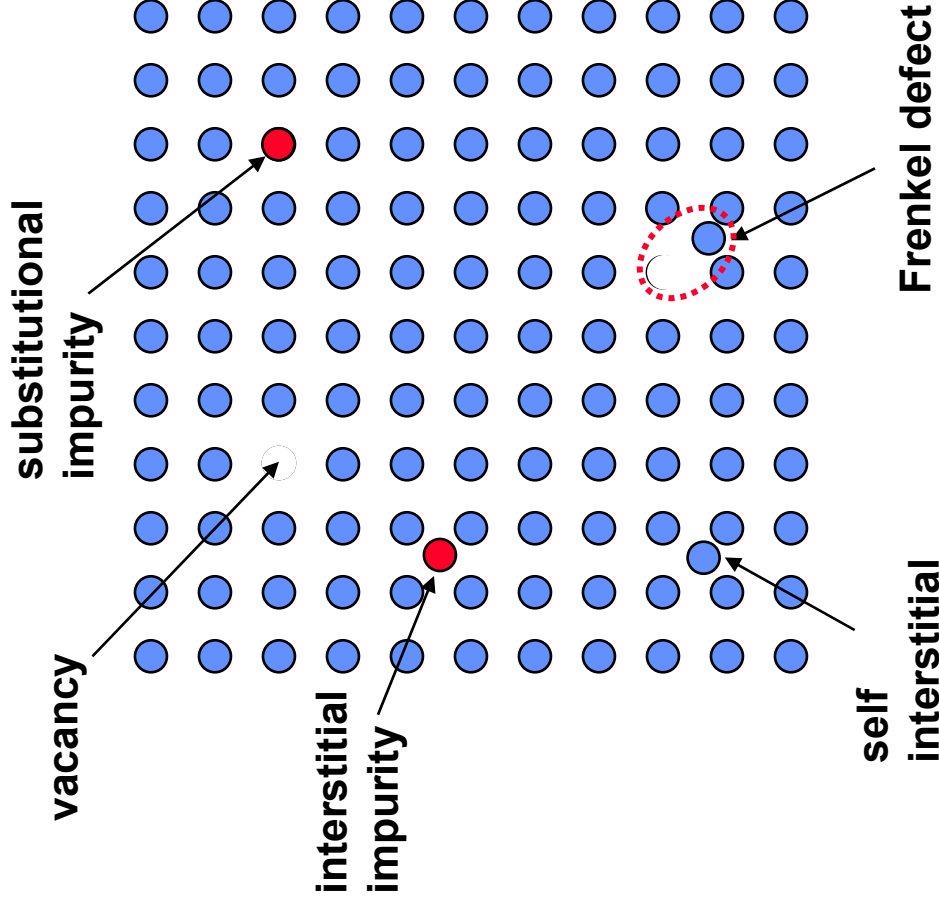
$$n \cong N_{\text{atomic}} e^{-E/kT}$$

- $E_{\text{formation}} \sim 2 \text{ eV}$
 - $T = 300\text{K}: n \sim 0$
 - $T = 1300\text{K}: n \sim 10^{13}$

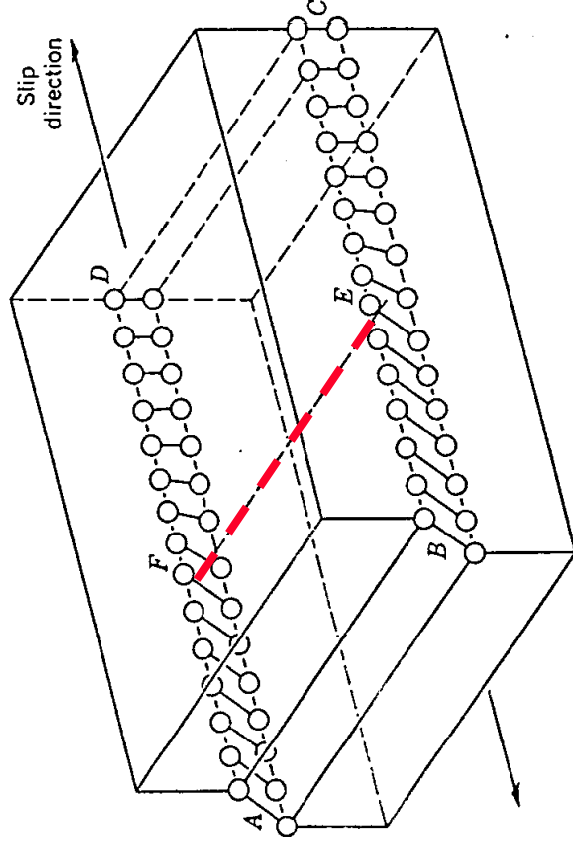
- vacancy-interstitial pair: Frenkel defect

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

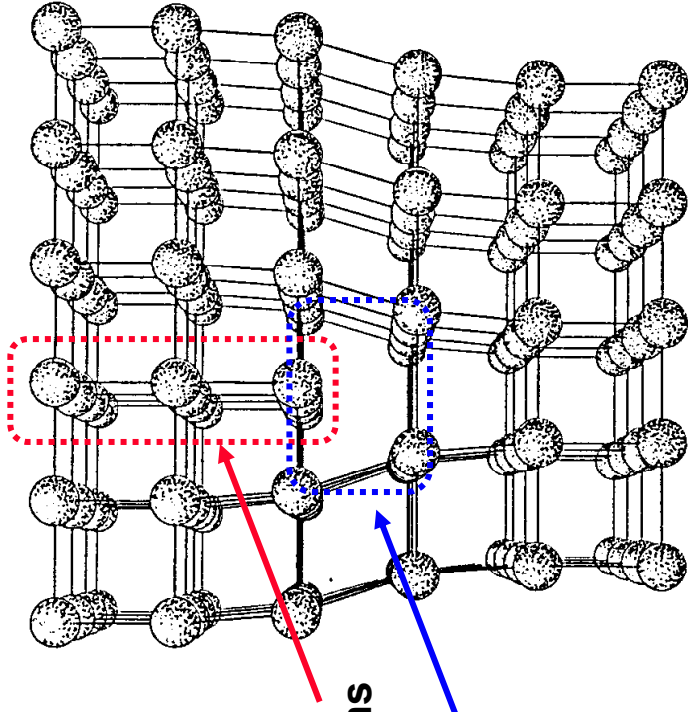
- $E_{\text{formation}} \sim 1 \text{ eV}$
 - $T = 300\text{K}: n \sim 10^{13}$
 - $T = 1300\text{K}: n \sim 10^{20}$



Edge Dislocations



\overline{EF} is
dislocation
line



- **one dimensional defect**

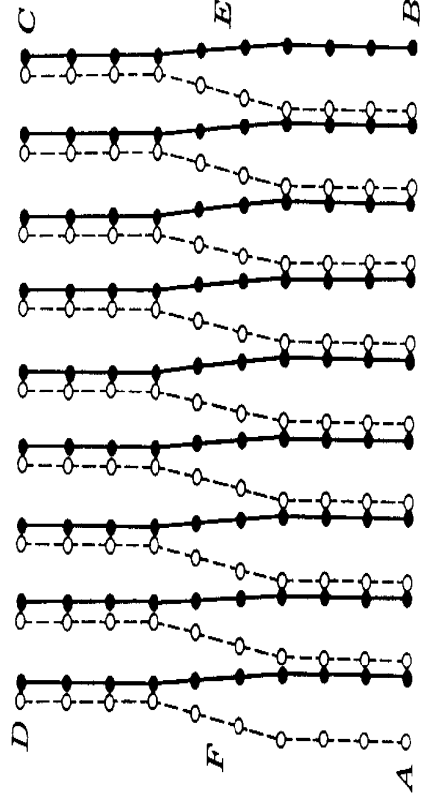
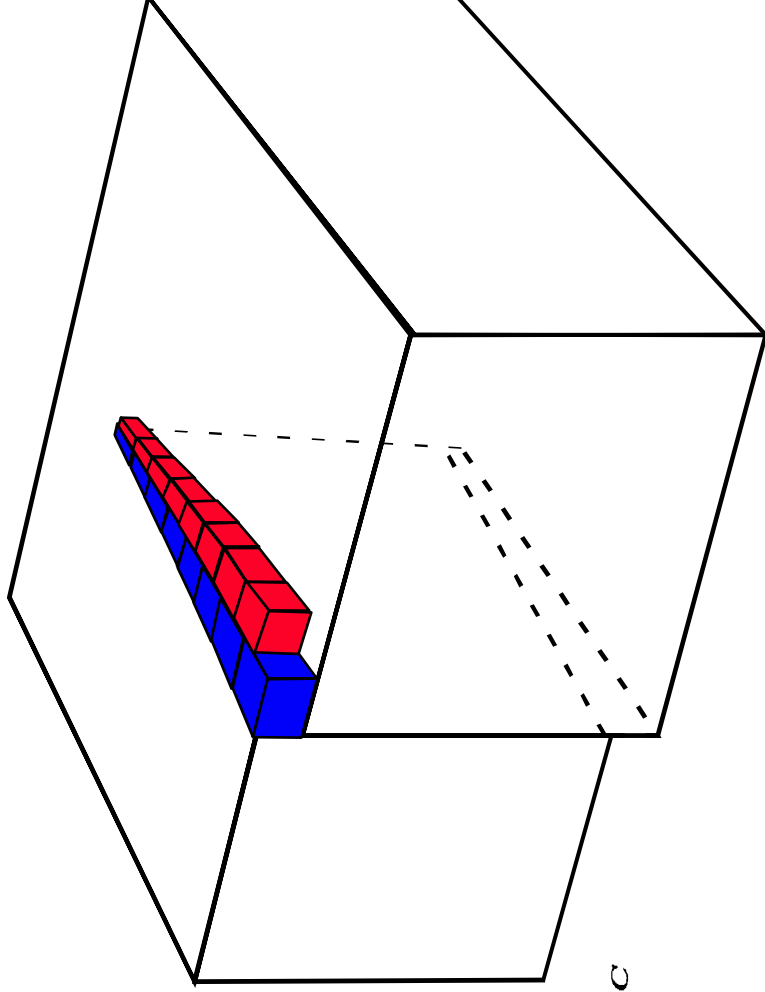
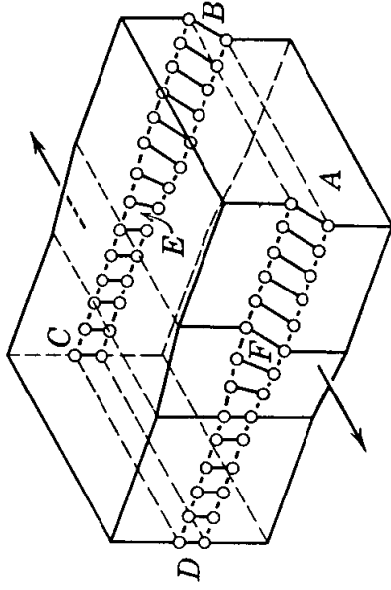
“extra” plane of atoms

- **formation energy is high, concentration usually low**

dislocation

from Kittel, p. 591

Screw Dislocation (1-d defect)



- screw dislocations are most commonly formed during crystal growth

Stacking arrangement and stacking faults

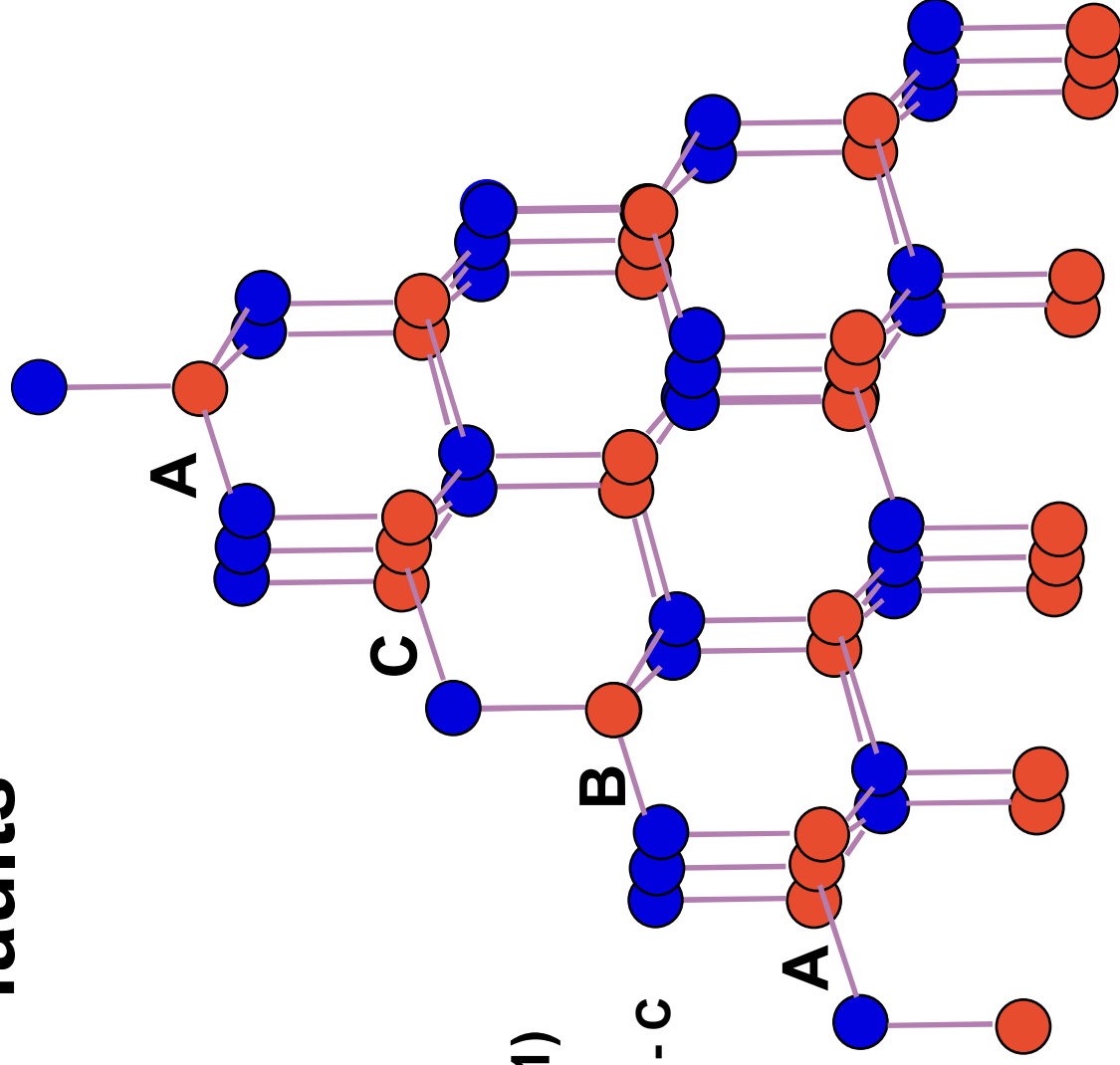
- layer ordering:

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

