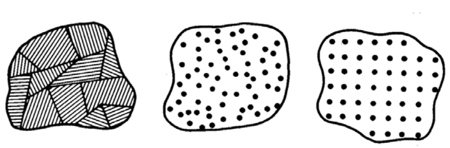
EE 116 Lecture 3

Atoms and Crystals

- Book: https://truenano.com/PSD20
- Intro and Review:
  - Read → Chapter 0.1-0.4
  - Scan and Review → Chapter 1 (*some* Phys 43, 45, 70 concepts)
- This lecture → Read 2.1 and 2.2

Crystal Lattices:

- Periodic arrangement of atoms
- Repeated unit cells (solid-state)
- Stuffing atoms into unit cells
- Diamond (Si) and zinc blende (GaAs) crystal structures
- Crystal planes
- Calculating densities



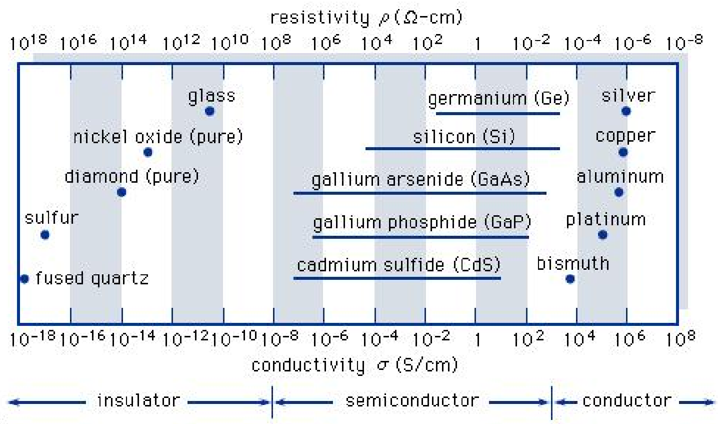
polycrystalline amorphous crystalline

IIB	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
	13 Al	14 Si	15 P	16 S
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te

- Some properties of semiconductors:

		E_g (ev)	μ_n (cm^2/V-s)	μ_p (cm^2/V-s)	m^*_n/m_o (m_l, m_t)	m^*_p/m_o (m_{lh}, m_{hh})	a (Å)	ϵ_r	Density (g/cm^3)	Melting point (°C)
Si	(i/D)	1.11	1350	480	0.98, 0.19	0.16, 0.49	5.43	11.8	2.33	1415
Ge	(i/D)	0.67	3900	1900	1.64, 0.082	0.04, 0.28	5.65	16	5.32	936
SiC (α)	(i/W)	2.86	500	—	0.6	1.0	3.08	10.2	3.21	2830
AlP	(i/Z)	2.45	80	—	—	0.2, 0.63	5.46	9.8	2.40	2000
AlAs	(i/Z)	2.16	1200	420	2.0	0.15, 0.76	5.66	10.9	3.60	1740
AlSb	(i/Z)	1.6	200	300	0.12	0.98	6.14	11	4.26	1080
GaP	(i/Z)	2.26	300	150	1.12, 0.22	0.14, 0.79	5.45	11.1	4.13	1467
GaAs	(d/Z)	1.43	8500	400	0.067	0.074, 0.50	5.65	13.2	5.31	1238
GaN	(d/Z, W)	3.4	380	—	0.19	0.60	4.5	12.2	6.1	2530
GaSb	(d/Z)	0.7	5000	1000	0.042	0.06, 0.23	6.09	15.7	5.61	712
InP	(d/Z)	1.35	4000	100	0.077	0.089, 0.85	5.87	12.4	4.79	1070
InAs	(d/Z)	0.36	22600	200	0.023	0.025, 0.41	6.06	14.6	5.67	943
InSb	(d/Z)	0.18	10^5	1700	0.014	0.015, 0.40	6.48	17.7	5.78	525

- Where crystalline semiconductors fit in (electrically):



- The periodic lattice:

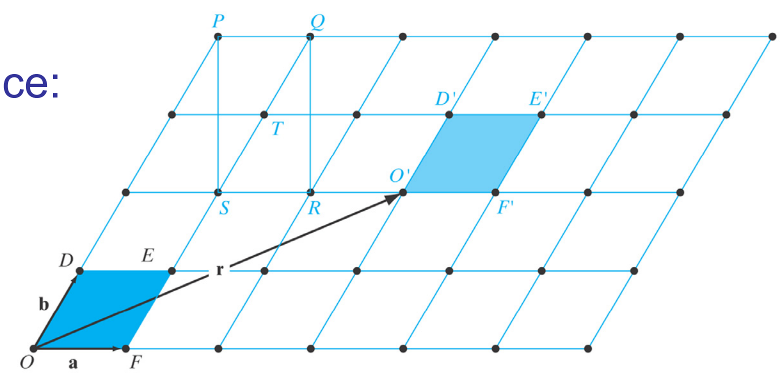
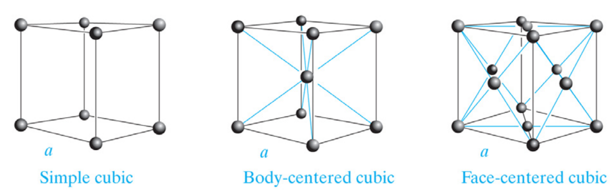


Figure 1.2

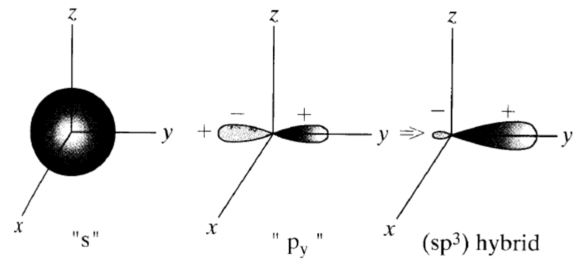
A two-dimensional lattice showing translation of a unit cell by $\mathbf{r} = 3\mathbf{a} + 2\mathbf{b}$.

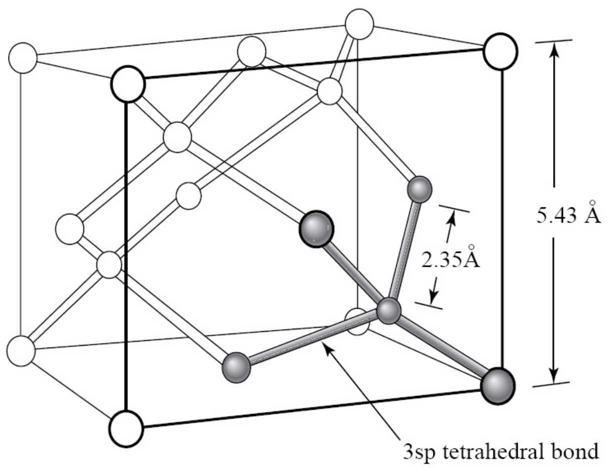
- Stuffing atoms into unit cells:
  - How many atoms per unit cell?
  - Avogadro's number: N_A = # atoms / mole
  - Atomic mass: A = grams / mole
  - Atom counting in unit cell: atoms / cm^3
  - How do you calculate density?



The Silicon lattice:

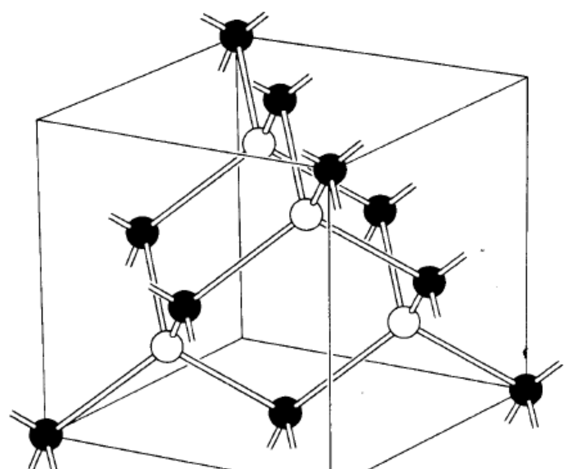
- Si atom: 14 electrons occupying lowest 3 energy levels:
  - 1s, 2s, 2p orbitals filled by 10 electrons
  - 3s, 3p orbitals filled by 4 electrons
- Each Si atom has four neighbors
- "Diamond lattice"
- How many atoms per unit cell?





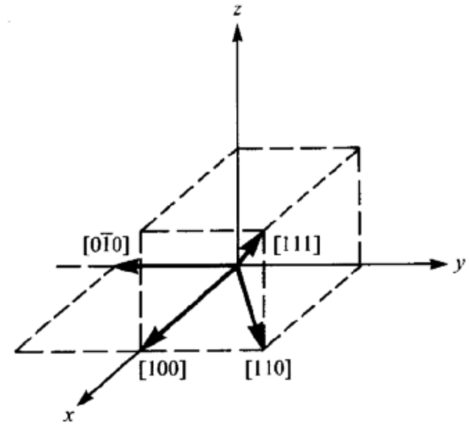
Zinc-blende lattice (ZnS, GaAs, AlAs, InP):

- Two intercalated fcc lattices



IIB	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
	13 Al	14 Si	15 P	16 S
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te

- Crystallographic notation

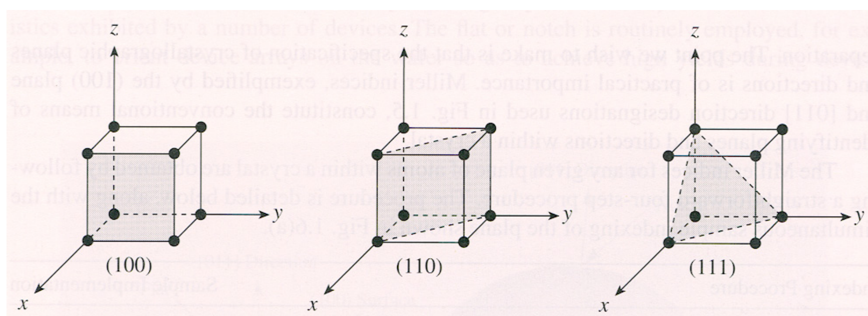


Sample direction vectors and their corresponding Miller indices.

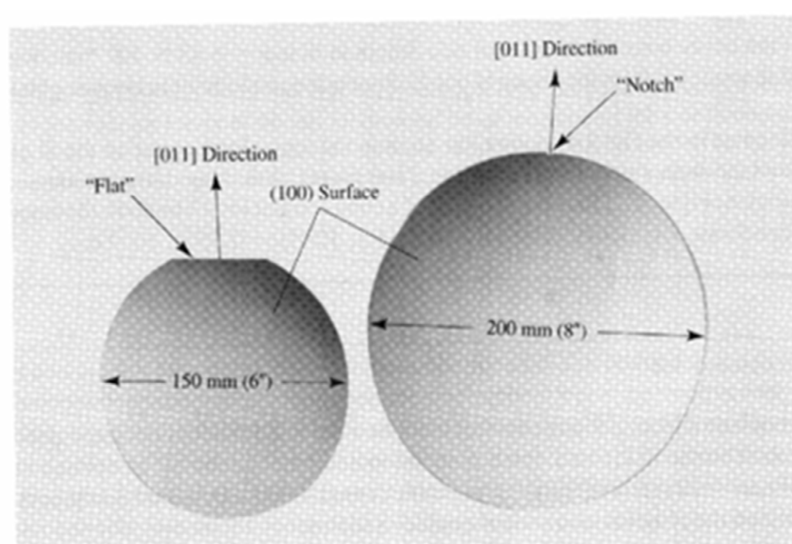
Notation	Interpretation
(*h k l*)	crystal plane
{ *h k l* }	equivalent planes
[*h k l*]	crystal direction
< *h k l* >	equivalent directions

***h*: inverse *x*-intercept of plane**
***k*: inverse *y*-intercept of plane**
***l*: inverse *z*-intercept of plane**

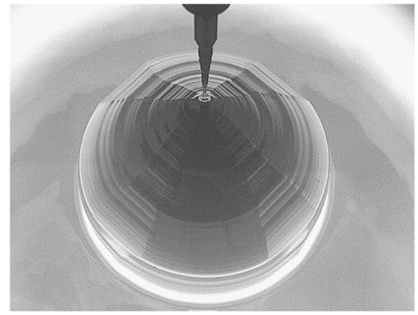
- Crystallographic planes and Si wafers



- Si wafers usually cut along {100} plane with a notch or flat side to orient the wafer during fabrication



- Where do (pure) Si wafers come from?
  - Read sections 1.3-1.4 in Streetman book
  - Take EE 212
  - Really short answer:



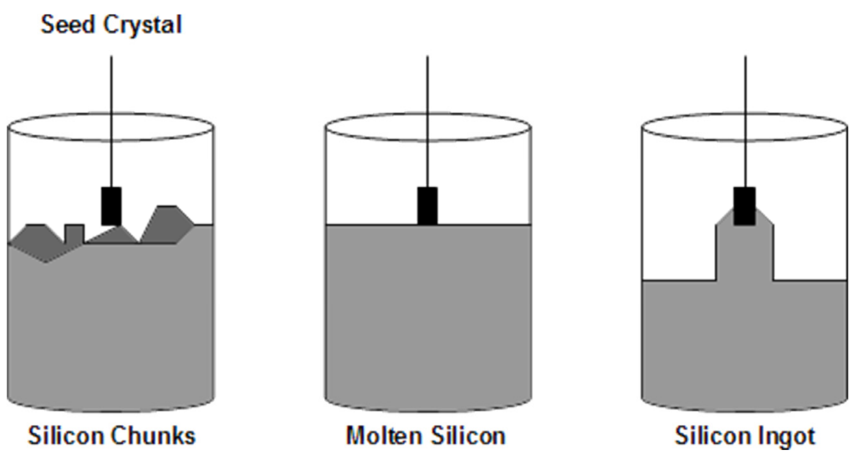
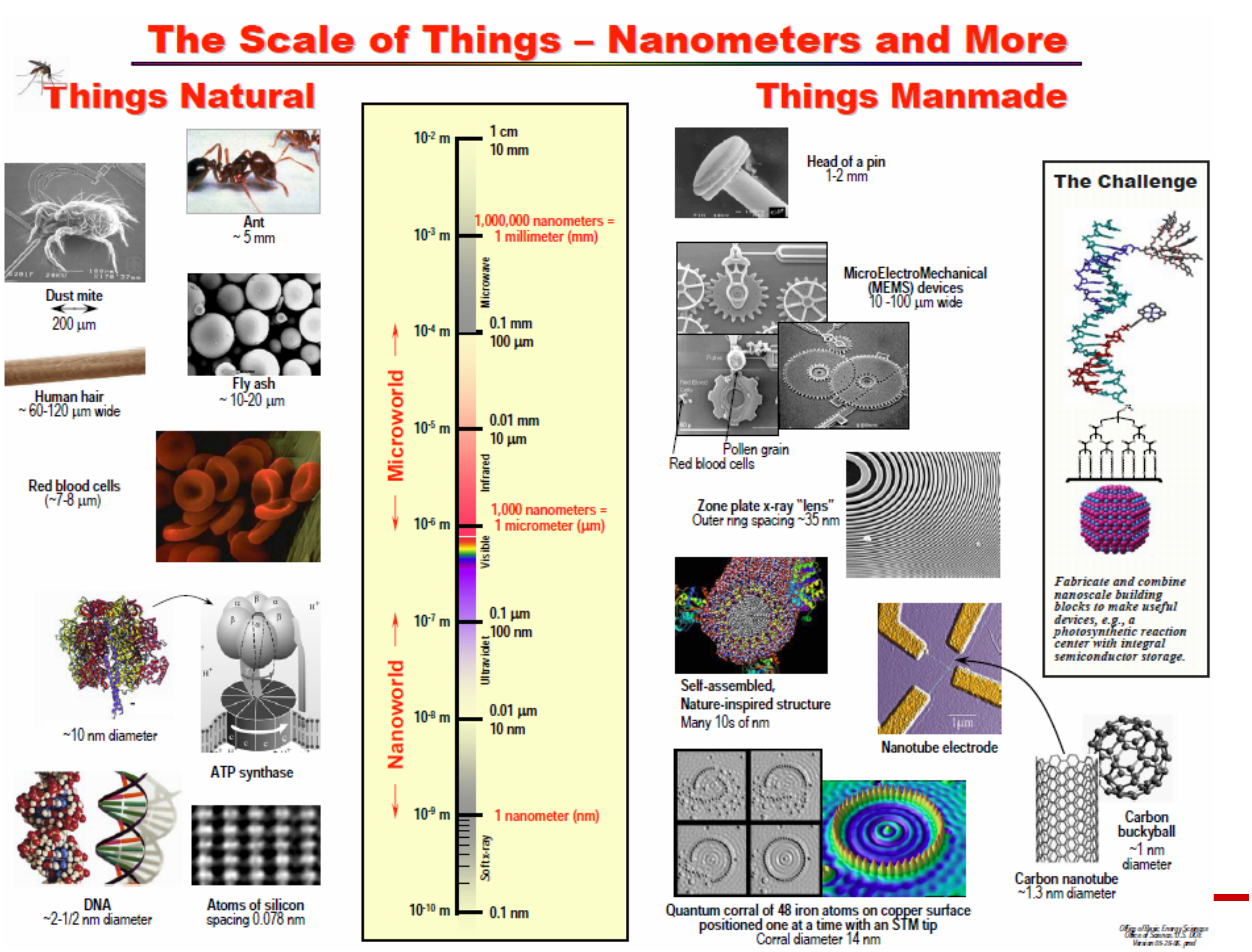


Image sources: Wikipedia

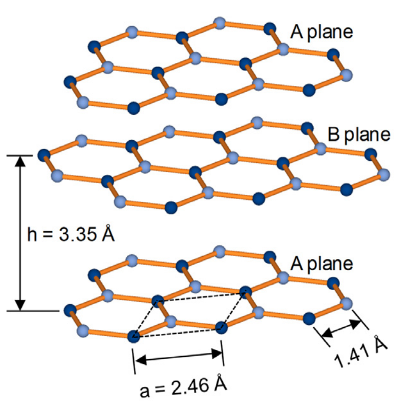


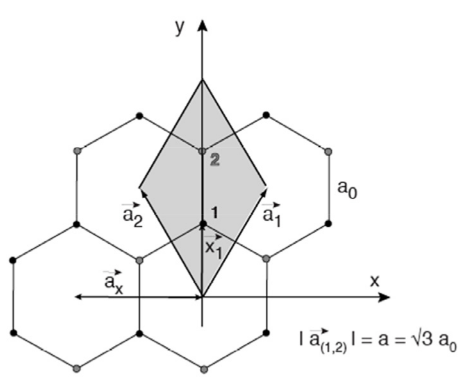
EE 116 Lecture 4
Bonds and Energy Bands

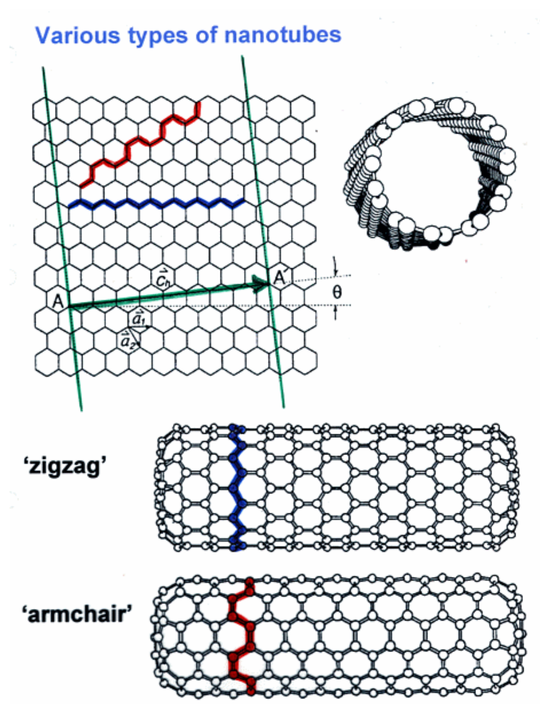
- Book: https://truenano.com/PSD20

- Read:
  - Ch. 1.2.4 (Bohr model)
  - Ch. 1.2.5 and 1.2.5.2 (Schrödinger equation and quantum well)
  - Ch. 2.3 up to 2.3.3.2
  - Ch. 2.3.4 and 2.3.5

- Graphite (~pencil lead) = parallel sheets of graphene
- Carbon nanotube = rolled up sheet of graphene







- The Bohr model of the (isolated) Si atom (N. Bohr, 1913):

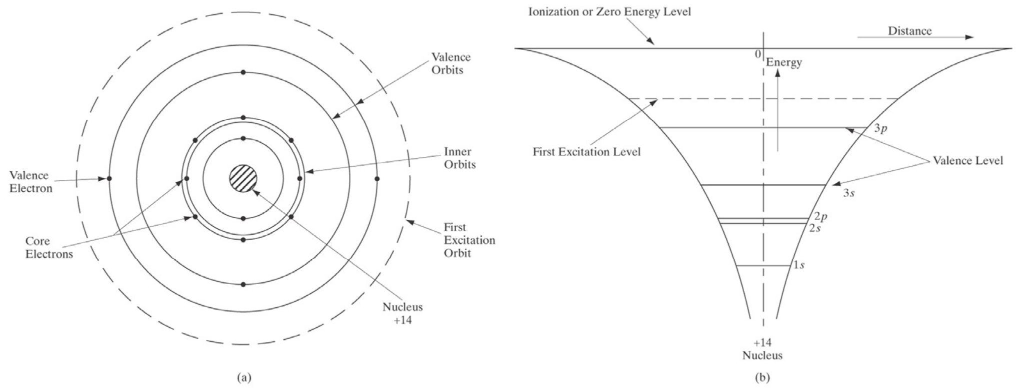


Figure 2.8

Electronic structure and energy levels in a Si atom: (a) The orbital model of a Si atom showing the 10 core electrons (**n** = 1 and 2), and the 4 valence electrons (**n** = 3); (b) energy levels in the coulombic potential of the nucleus are also shown schematically.

- Note: inner shell electrons *screen* outer shell electrons from the positive charge of the nucleus (outer less tightly bound)

- Bohr model: $E_B = -\frac{mq^4}{2(4\pi\varepsilon\hbar\mathbf{n})^2} = -\frac{13.6}{\mathbf{n}^2}\ \text{eV}$

Quantum theory on two slides:

1) Key result of quantum mechanics (E. Schrödinger, 1926):

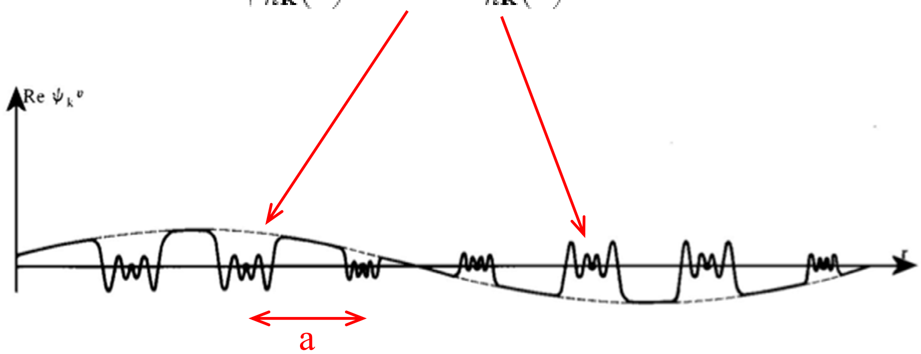
- Particle/wave in a <u>single</u> (potential energy) box
- Discrete, separated energy levels

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

2) Key result of wave mechanics (F. Bloch, 1928):

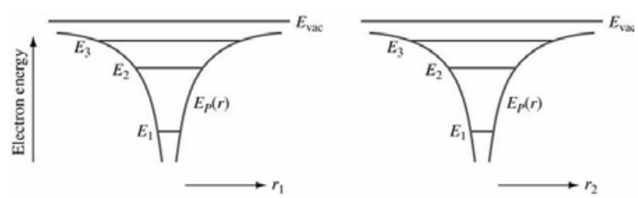
- Plane wave in a periodic potential (Kronig-Penney model)
- Wave momentum k only unique up to 2π/a
- Only certain electron energies allowed, but those can propagate unimpeded (theoretically), as long as lattice spacing is “perfectly” maintained!!!
- But, resistance introduced by: __________ and __________

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}).$$

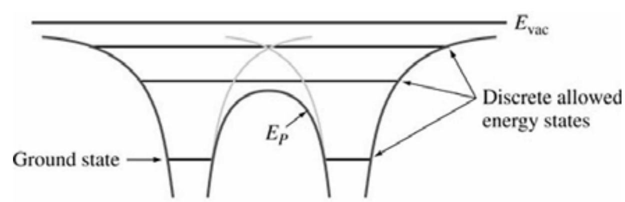


see: http://www.chembio.uoguelph.ca/educmat/chm729/wscells/wigner.htm

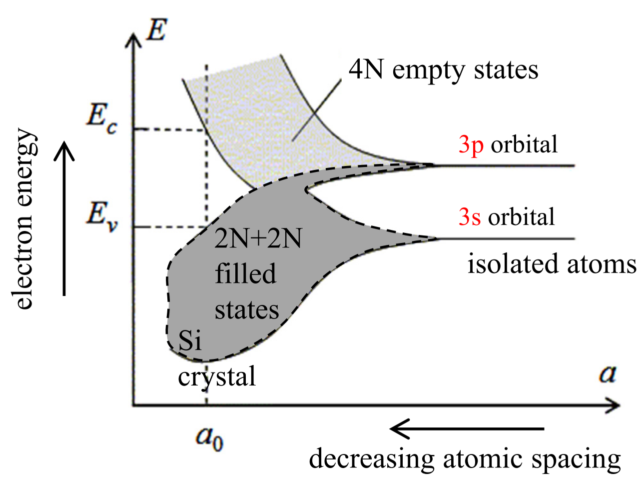
- Energy levels when atoms are far apart:



- Energy levels when atoms are close together (potentials interact):



- Energy levels from discrete atoms to crystal lattice:



- Energy states of Si atom expand into energy bands of Si lattice
- Lower bands are filled with electrons, higher bands are empty in a semiconductor
- The highest filled band = ___________ band
- The lowest empty band = ___________ band
- Insulators?
- Metals?

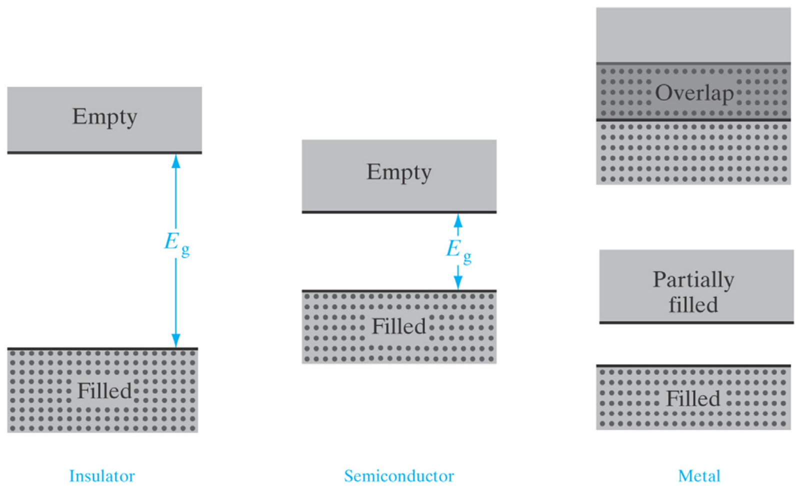
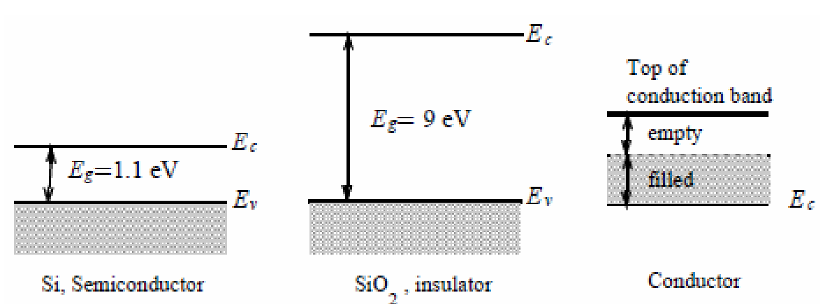
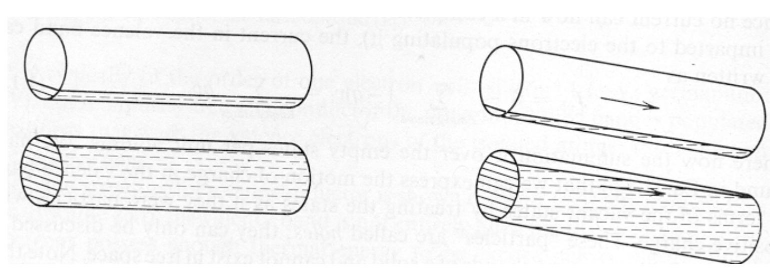


Figure 3.4

Typical band structures at 0 K.

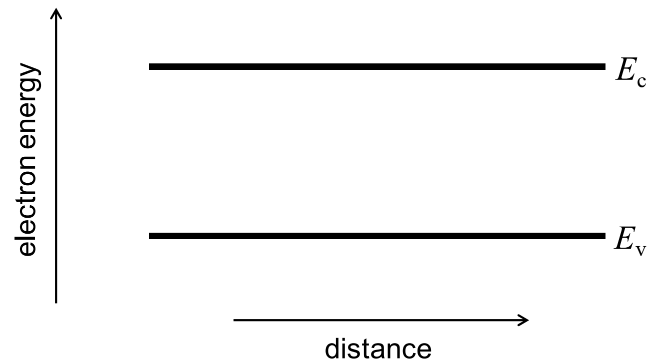


- Band structure explains why SiO_2 (diamond, etc) is insulating, silicon is semiconducting, copper is a metal
- *For electrons to be accelerated in an electric field they must be able to move into new, unoccupied energy states.*



- Water bottle flow analogy (empty vs. full)
- So, what is a hole then?

- In devices we usually draw:



- Simplified version of energy band model, indicating
  - Top edge of valence band (E_V)
  - Bottom edge of conduction band (E_C)
  - Their separation, i.e. band gap energy (E_G)

EE 116 Lecture 5

Energy Bands, Temperature, Effective Mass

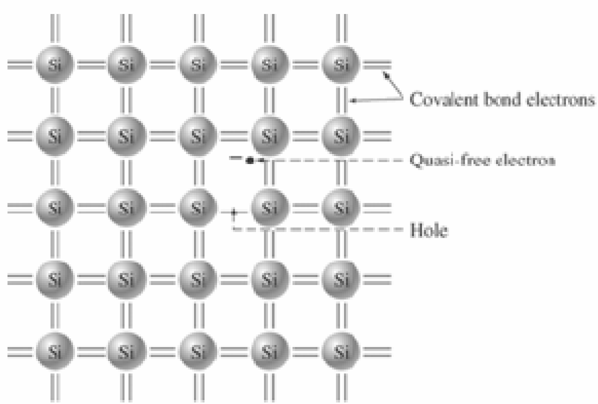
- Book: https://truenano.com/PSD20

- Skim 2.3.6 and 2.3.7
- Begin reading 2.7

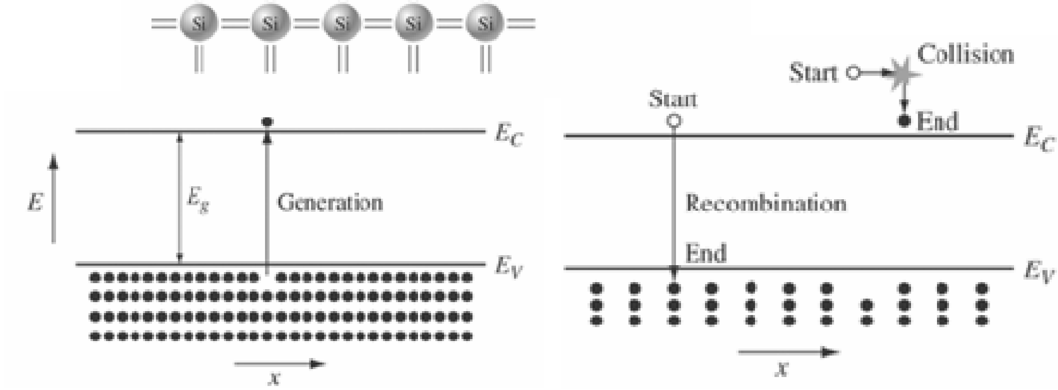
- Typical semiconductor band gaps (E_G) between 0-3 eV
  - GaAs → $E_G \approx 1.4$ eV
  - Si → $E_G \approx 1.1$ eV
  - Ge → $E_G \approx 0.7$ eV
- For more, see table back in Lecture 3
- Insulator band gaps > 5 eV → SiO_2 $E_G = 9$ eV

- What is an eV?
- Where are all electrons at T=0 K?
- Do either insulators or semiconductors conduct at 0 K?
- What about at T=300 K?

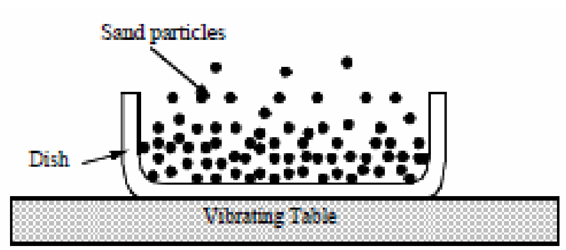
bond picture:
(here 2-D)



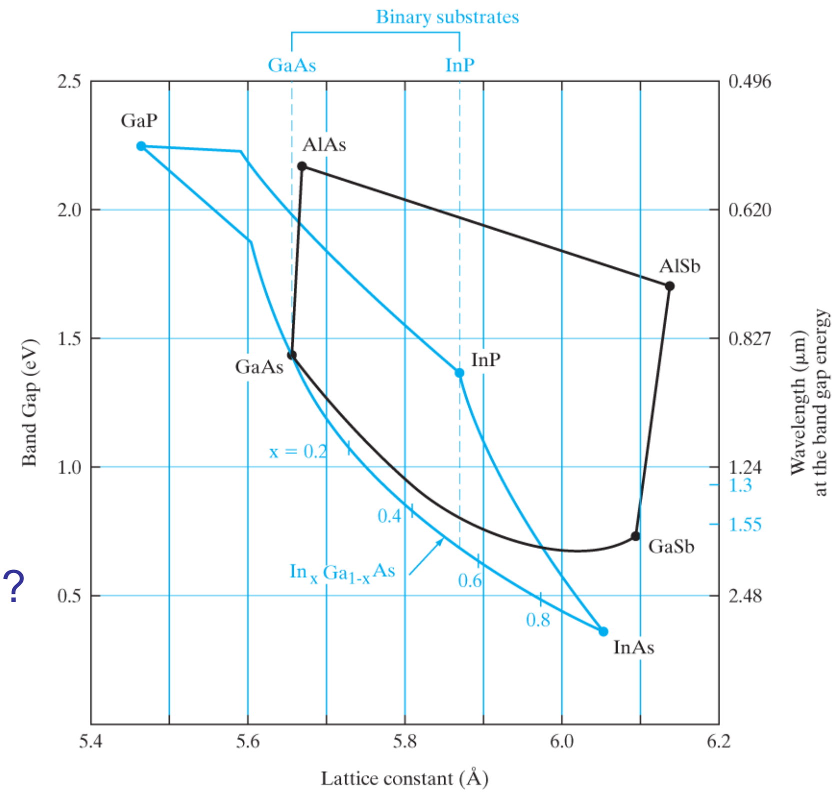
band picture:



mechanical analogy:

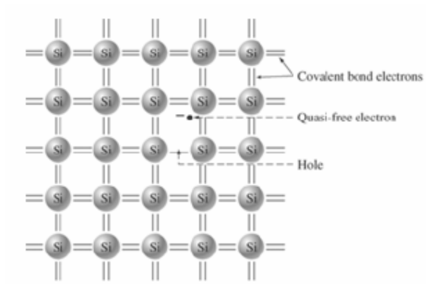


- How do band gaps vary with lattice size? (is there a trend?)



- How do band gaps vary with temperature?

- Short recap, so we are comfortable switching between:
  - Bond picture



  - Band picture vs. x
  - Band picture vs. k

- Let’s combine energy bands vs. k and vs. x:

- Note what is *potential*, *kinetic*, and *total* energy

- Note which way energy of *holes* increases

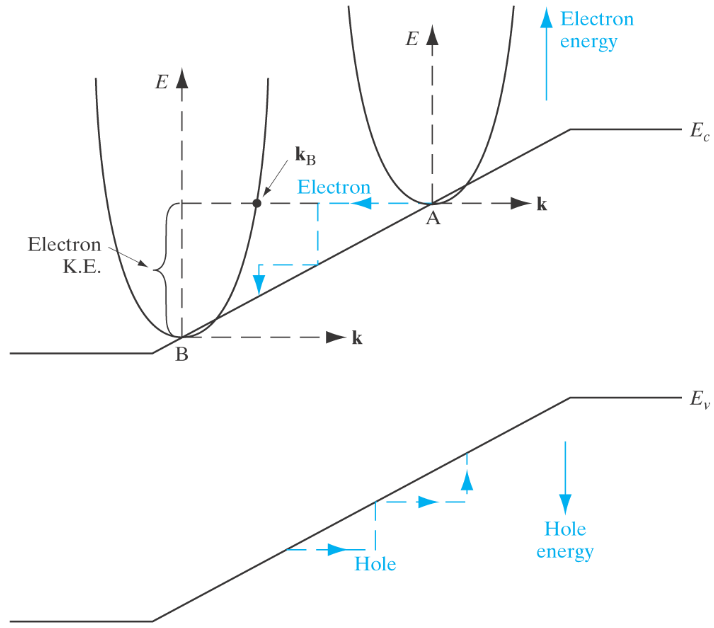
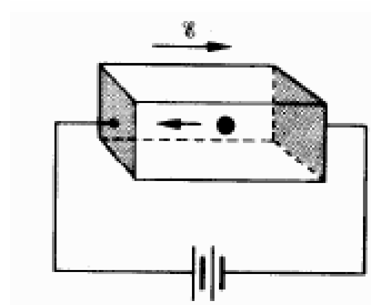


Figure 3.9

Superimposition of the (E,**k**) band structure on the E-versus-position simplified band diagram for a semiconductor in an electric field. Electron energies increase going up, while hole energies increase going down. Similarly, electron and hole wave vectors point in opposite directions and these charge carriers move opposite to each other, as shown.



- Electrons (or holes) as moving particles:

- Newton’s law still applies: $F = m^*a$
- Where m^* = the “effective mass” of the particle, which includes all the complex influences of the crystal potential on the motion of the electron (or hole).

- Acceleration?
  - For electrons: For holes:

- Effective mass values? Fractions of m_0 (see tables).
  - Sometimes depend on direction of motion in the crystal.
  - E.g. for electrons in Si: $m_l = 0.98m_0$, $m_t = 0.19m_0$
  - Can also depend on particle location in the band (bottom, top, edge, “light” band vs. “heavy” band).
  - Values are typically given at the bottom of C-band for electrons, top of V-band for holes.

- Q: What is the meaning of the energy band *slope* in the E-x band diagram picture?

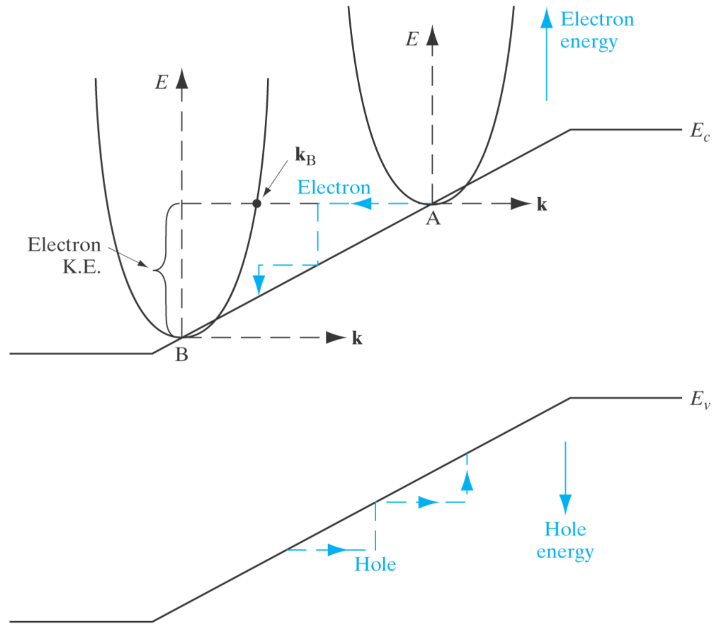


Figure 3.9

Superimposition of the $(E,\mathbf{k})$ band structure on the *E*-versus-position simplified band diagram for a semiconductor in an electric field. Electron energies increase going up, while hole energies increase going down. Similarly, electron and hole wave vectors point in opposite directions and these charge carriers move opposite to each other, as shown.