Trends in III-V and II-VI Compounds

Larger atoms, weaker bonds, smaller U, smaller E_g, higher μ, more costly!

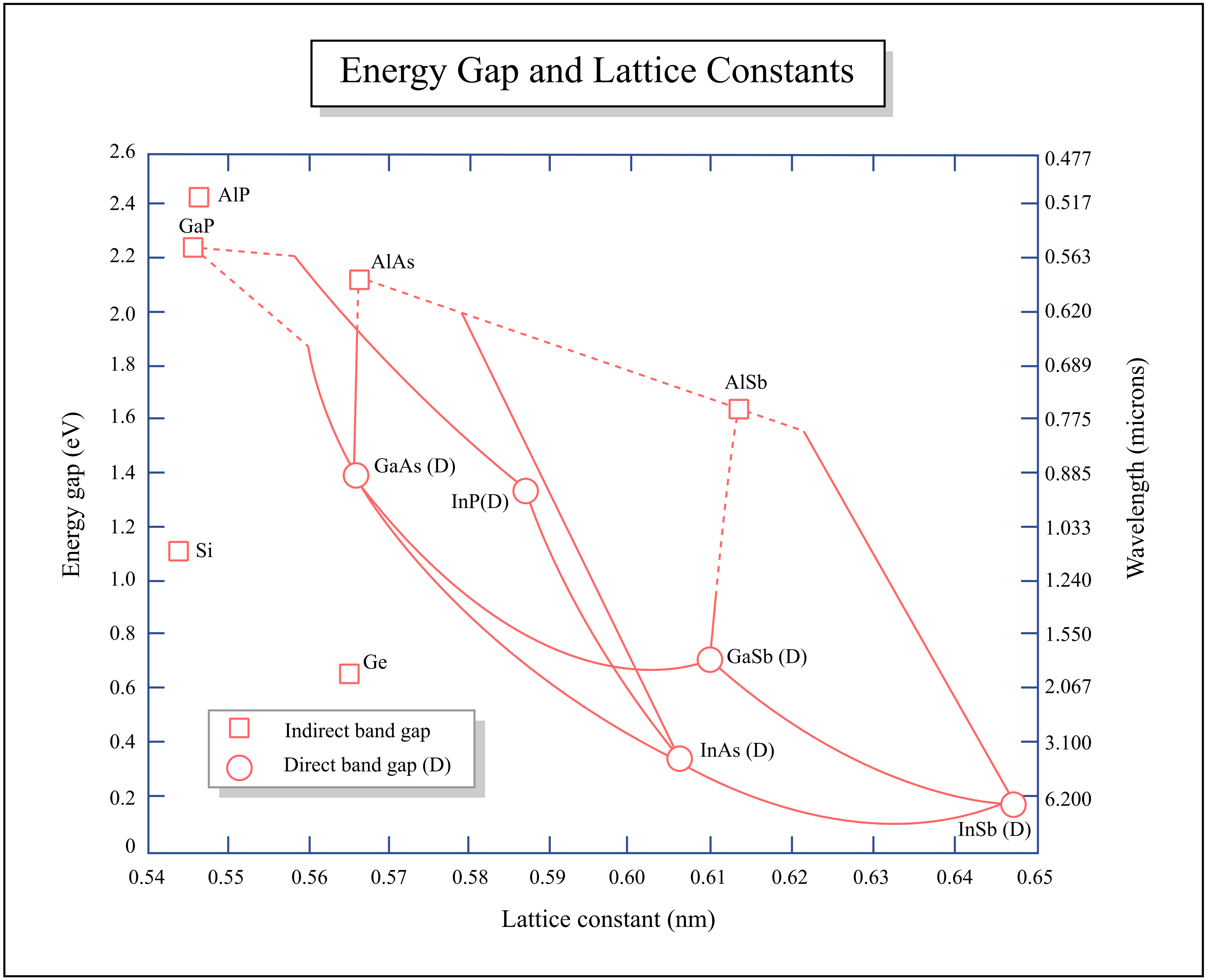
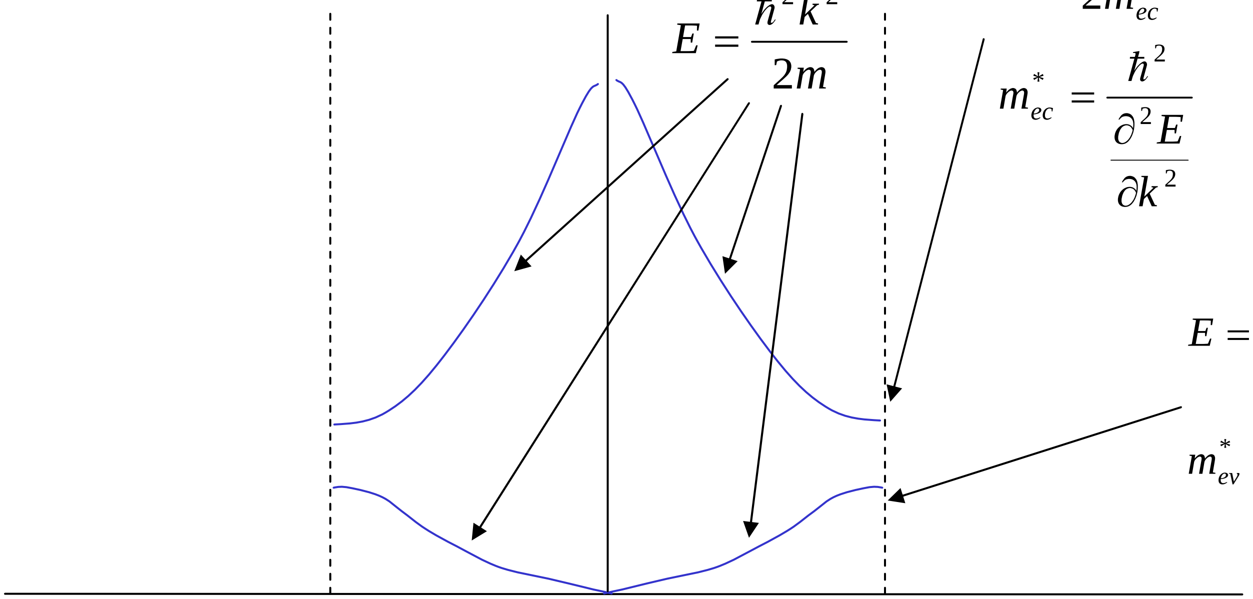


Figure by MIT OpenCourseWare.

Properties of non-free e-

- Electrons near the diffraction condition are not approximated as free
- Their properties can still be viewed as free e- if an ‘effective mass’ m* is used



$$E = \frac{\hbar^2 k^2}{2m}$$

$$E = \frac{\hbar^2 k^2}{2m_{ec}^*}$$

$$m_{ec}^* = \frac{\hbar^2}{\frac{\partial^2 E}{\partial k^2}}$$

$$E = \frac{\hbar^2 k^2}{2m_{ev}^*}$$

$$m_{ev}^* = \frac{\hbar^2}{\frac{\partial^2 E}{\partial k^2}}$$

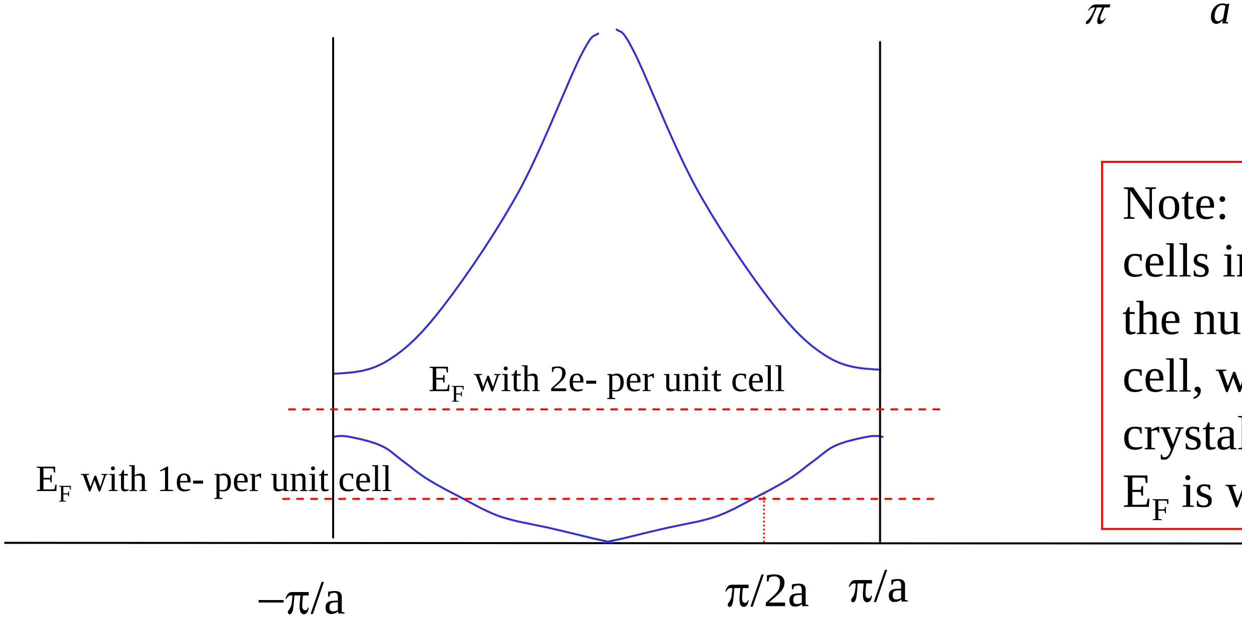
Note: These electrons have negative mass!

1-D Crystal Metals and Insulators

- How do band gaps affect properties of materials?
- Only electrons near E_F participate in properties
- If E_F is in the middle of the band, free e- and metallic behavior
- If E_F is near the band gap, changes in materials properties may occur
- Need to find out where E_F is!

$$N = \frac{2k_F L}{\pi} = \frac{2L}{a}$$

Where $k_F=\pi/a$ if we want to see how many electrons are in first band



Note: L/a is the number of unit cells in the 1-D crystal; therefore, the number of electrons per unit cell, which depends on n and the crystal structure, determine where E_F is with respect to the band gap

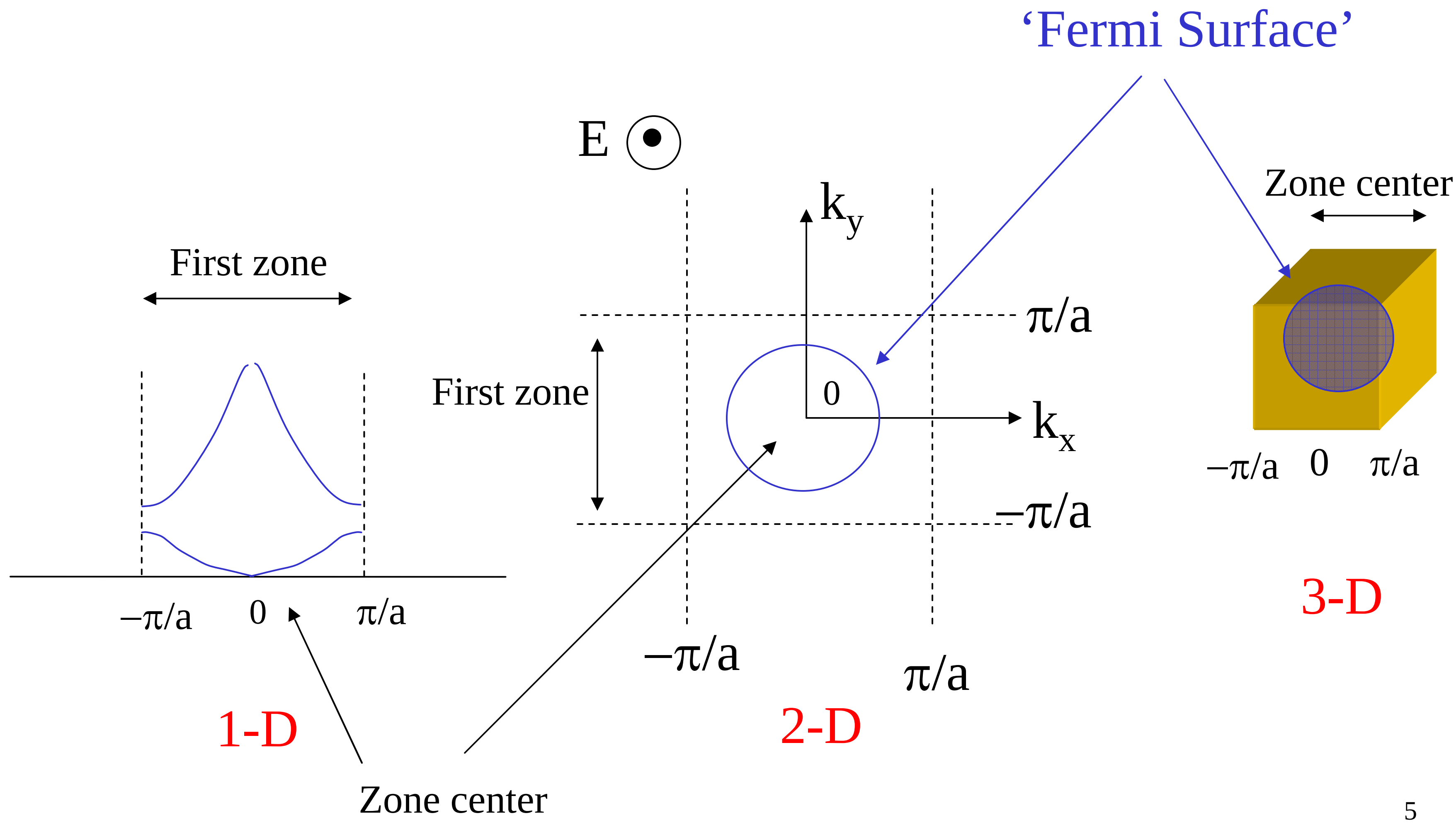
1-D Crystal Metals and Insulators

- 2e- per unit cell: E_F at band edge: 2 possibilities
  - Band gap >> kT: electrons at band max can not accept energy from electric fields; no conduction, *insulating behavior*
  - Band gap near kT: some thermal fluctuations large enough to allow population of second band; carriers are there, but less than for free e-, *semimetal*
- 1e- per unit cell: E_F in middle of band: free e-, *metallic*

Note: crystal structure (number of atoms per primitive cell) and valence (number of conduction electrons per atom), combined with band gap size, determine the electronic properties

Higher Dimensions (2 and 3-D)

- 1-D: $E(k_x)$; 2-D: $E(k_x,k_y)$; 3-D: $E(k_x,k_y,k_z)$



Metals and Insulators

- Covalent bonds, weak U seen by e-, with E_F being in mid-band area: free e-, *metallic*
- Covalent or slightly ionic bonds, weak U to medium U, with E_F near band edge
  - E_F in or near kT of band edge: *semimetal*
  - E_F in gap: *semiconductor*
- More ionic bonds, large U, E_F in very large gap, *insulator*

Insulators

- Very large band gaps=no conduction electrons at reasonable temperatures
- All electrons are bound
- Optical properties of insulators are derived from the electric field being able to temporarily move electrons: polarization
- We will return to the interaction of E-field with bound electrons in Dielectrics Section