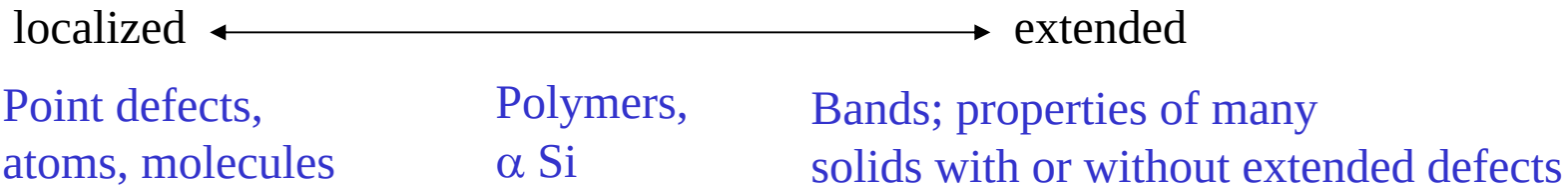
Remaining Issues

- Electron wave picture has fixed some thermal/electrical properties and electron velocity issues
- Still can not explain:
  - Hall coefficients
  - Colors of metals
  - Insulators, Semiconductors
- Can not ignore the ions (i.e. everything else but the valence electrons that we have been dealing with so far) any longer!
- Whatever we modify, can not change the electron wave picture that is now working well for many materials properties
- HOW DO THE VALENCE ELECTRON WAVES INTERACT WITH THE IONS AND THEIR POTENTIALS?

Improvements? What are ion cores doing...

- Scattering idea seems to work
- any effect of crystal (periodic) lattice?
- Diffraction
  - proves periodicity of lattice
  - proves electrons are waves
  - proves strong interaction between crystal and electrons (leads to band structures=semiconductors and insulators)
  - useful characterization technique
- Course: bias toward crystalline materials: many applications: materials related to either end of spectrum (atomic/molecular or crystalline)



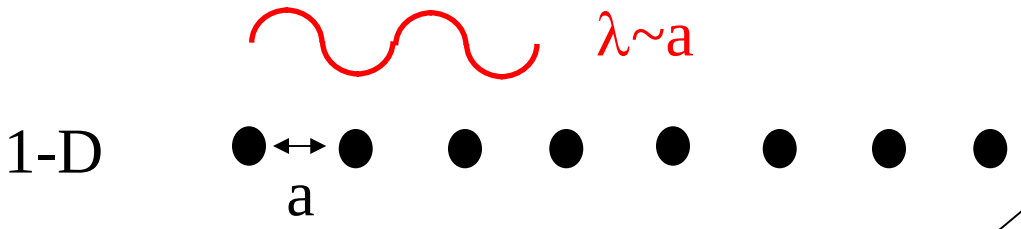
Diffraction is a useful characterization in all these materials

Electrons in a Periodic Potential

- Rigorous path: $H\Psi=E\Psi$
- We already know effect: DeBroglie and electron diffraction
- Unit cells in crystal lattice are 10^{-8} cm in size
- Electron waves in solid are $\lambda=h/p\sim10^{-8}$ cm in size
- Certain wavelengths of valence electrons will diffract!

Diffraction Picture of the Origin of Band Gaps

- Start with 1-D crystal again



$$n\lambda = 2d\sin\theta$$

d=a, sinθ=1

$$n\lambda = 2a$$

$$k = \frac{2\pi}{\lambda}$$

$$k = \frac{\pi n}{a}$$

Take lowest order, n=1, and consider an incident valence electron moving to the right

$$k_i = \frac{\pi}{a}; \psi_i = e^{i\frac{\pi}{a}x}$$

Reflected wave to left: $k_o = -\frac{\pi}{a}; \psi_o = e^{-i\frac{\pi}{a}x}$

$$\Delta k = k_i - k_o = \frac{2\pi}{a}$$

Total wave for electrons with diffracted wavelengths:

$$\psi = \psi_i \pm \psi_o$$

$$\psi_s = \psi_i + \psi_o = 2\cos\frac{\pi}{a}x$$

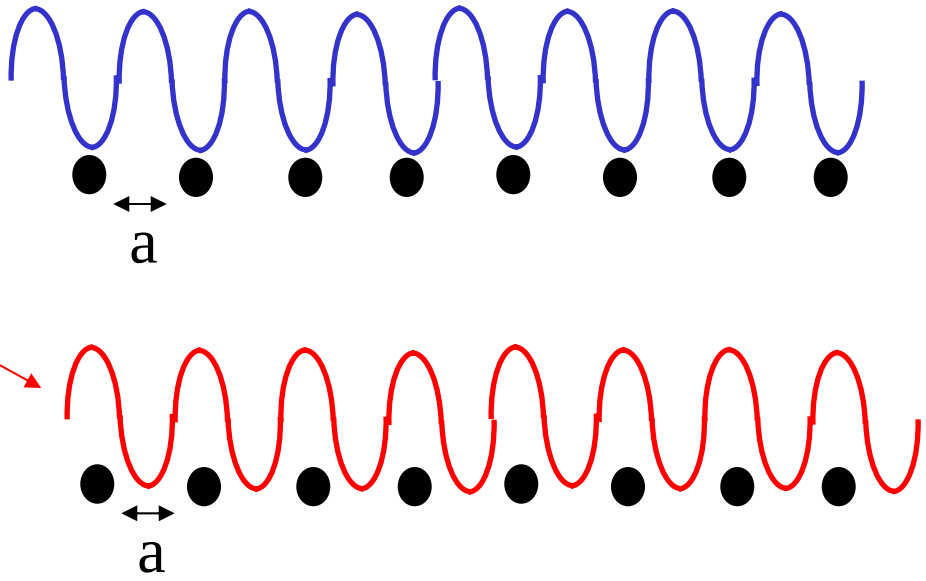
$$\psi_a = \psi_i - \psi_o = i2\sin\frac{\pi}{a}x$$

Diffraction Picture of the Origin of Band Gaps

Probability Density=probability/volume of finding electron=$|\psi|^2$

$$|\psi_a|^2 = 4\sin^2\frac{\pi}{a}x$$

$$|\psi_s|^2 = 4\cos^2\frac{\pi}{a}x$$



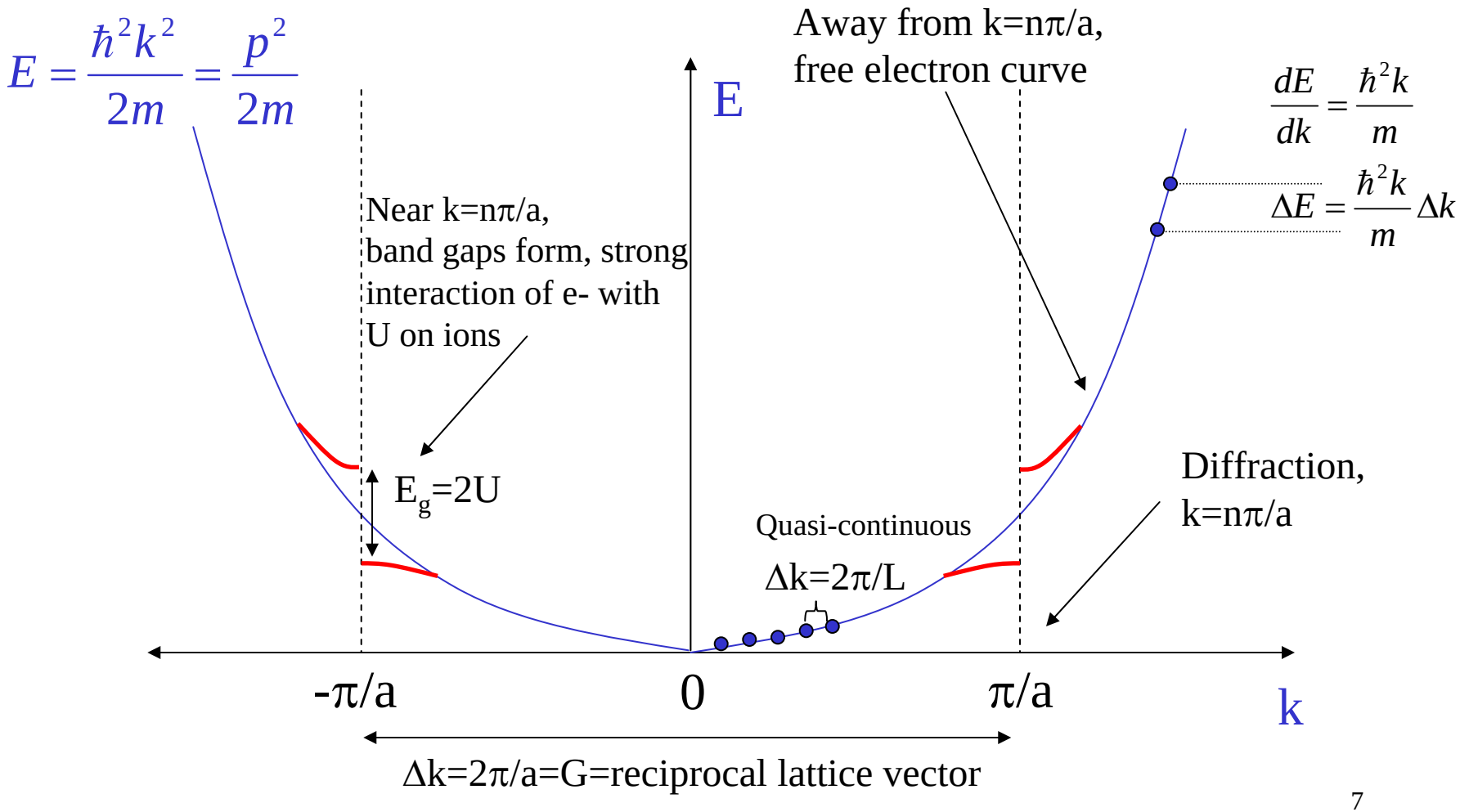
- Only two solutions for a diffracted wave
  - Electron density on atoms
  - Electron density off atoms
- No other solutions possible at this wavelength: no free traveling wave

Nearly-Free Electron Model

- Assume electrons with wave vectors (k's) far from diffraction condition are still free and look like traveling waves and see ion potential, U, as a weak background potential
- Electrons near diffraction condition have only two possible solutions
  - electron densities between ions, $E=E_{free}-U$
  - electron densities on ions, $E= E_{free}+U$
- Exact solution using $H\Psi=E\Psi$ shows that E near diffraction conditions is also parabolic in k, $E\sim k^2$

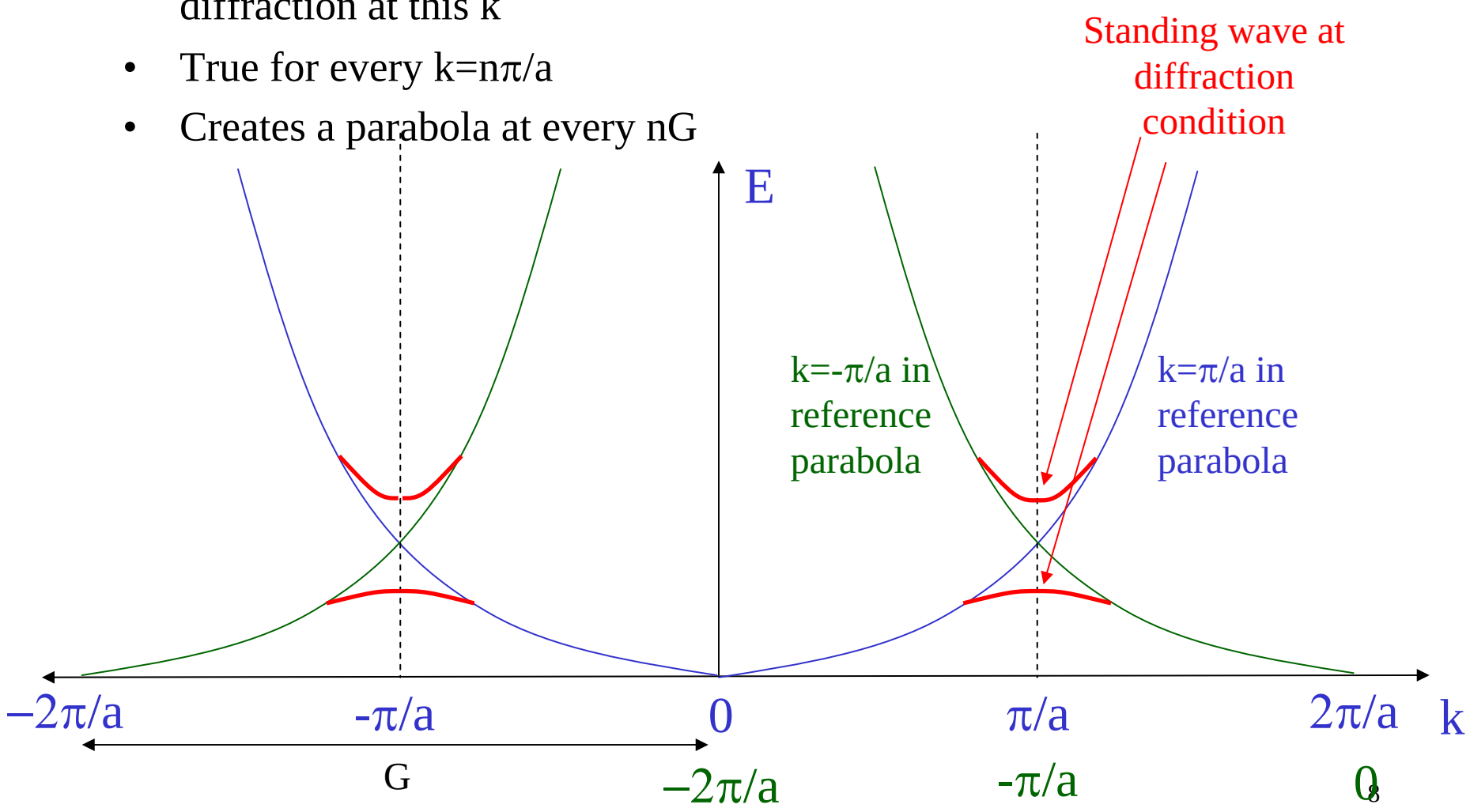
Nearly-Free Electron Model (still 1-D crystal)

- states



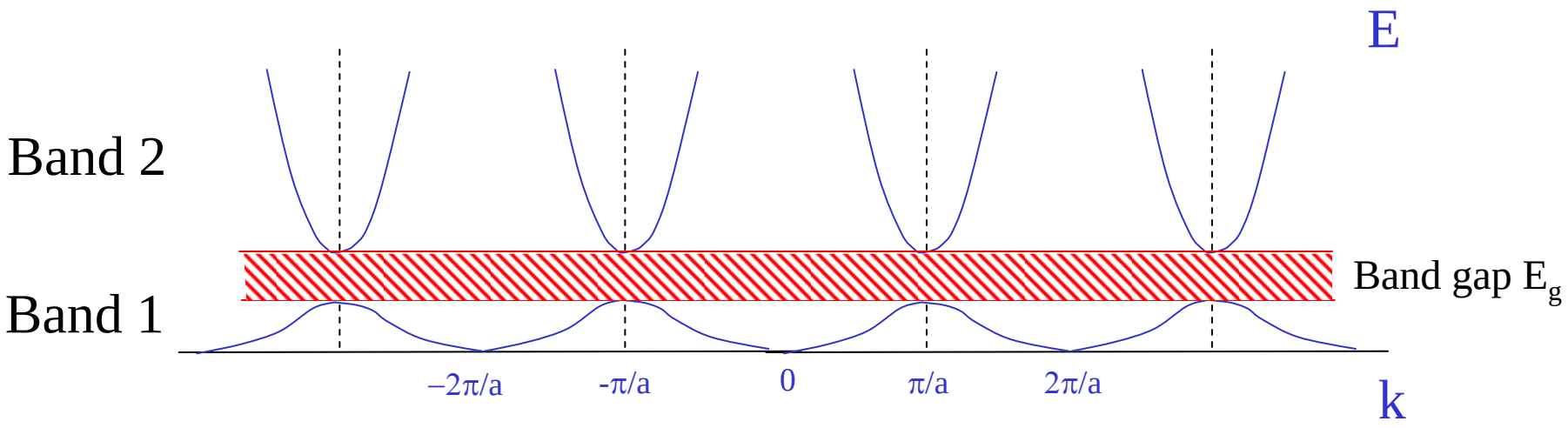
Consequences of Diffraction on E vs. k curves

- At k=π/a, there must be also a k=-π/a wave, since there is absolute diffraction at this k
- True for every k=nπ/a
- Creates a parabola at every nG



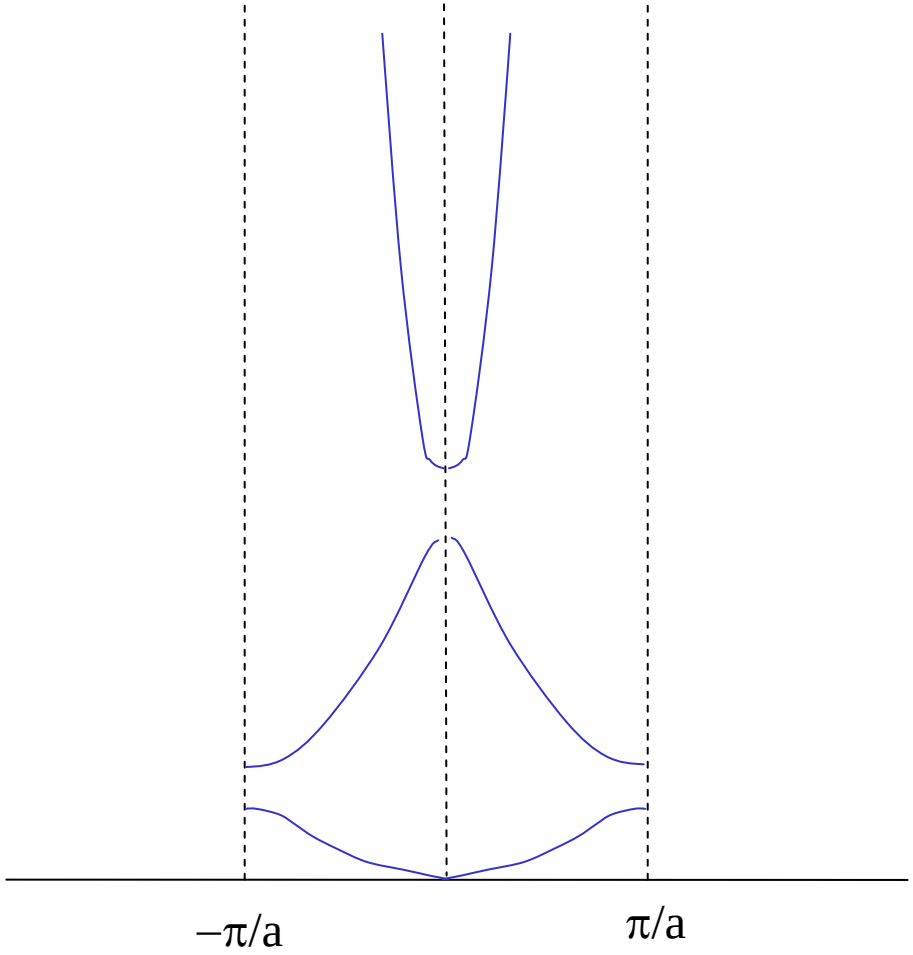
Extended-Zone Scheme

- Bands form, separated by band gaps
- Note redundancy: no need for defining k outside +-π/a region



Reduced-Zone Scheme

- Only show k=+-π/a since all solutions represented there



Real Band Structures

- GaAs: Very close to what we have derived in the nearly free electron model
- Conduction band minimum at k=0: Direct Band Gap

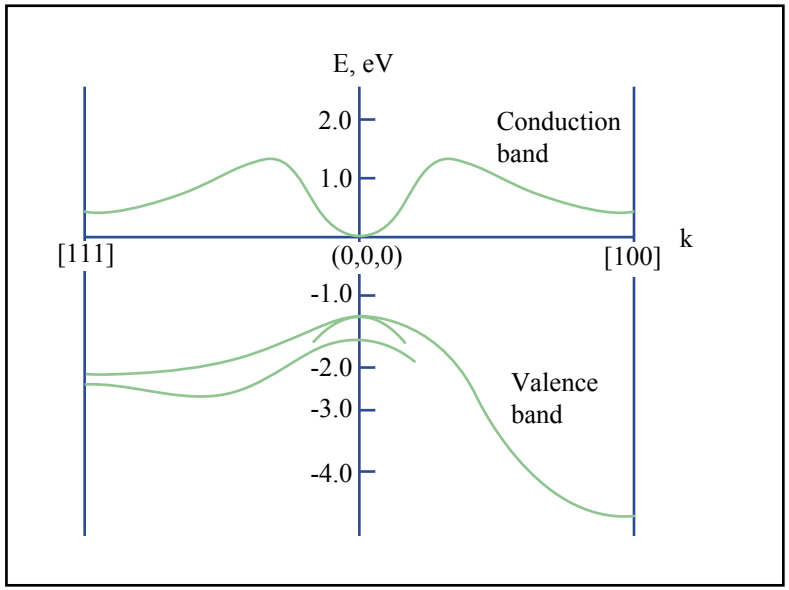
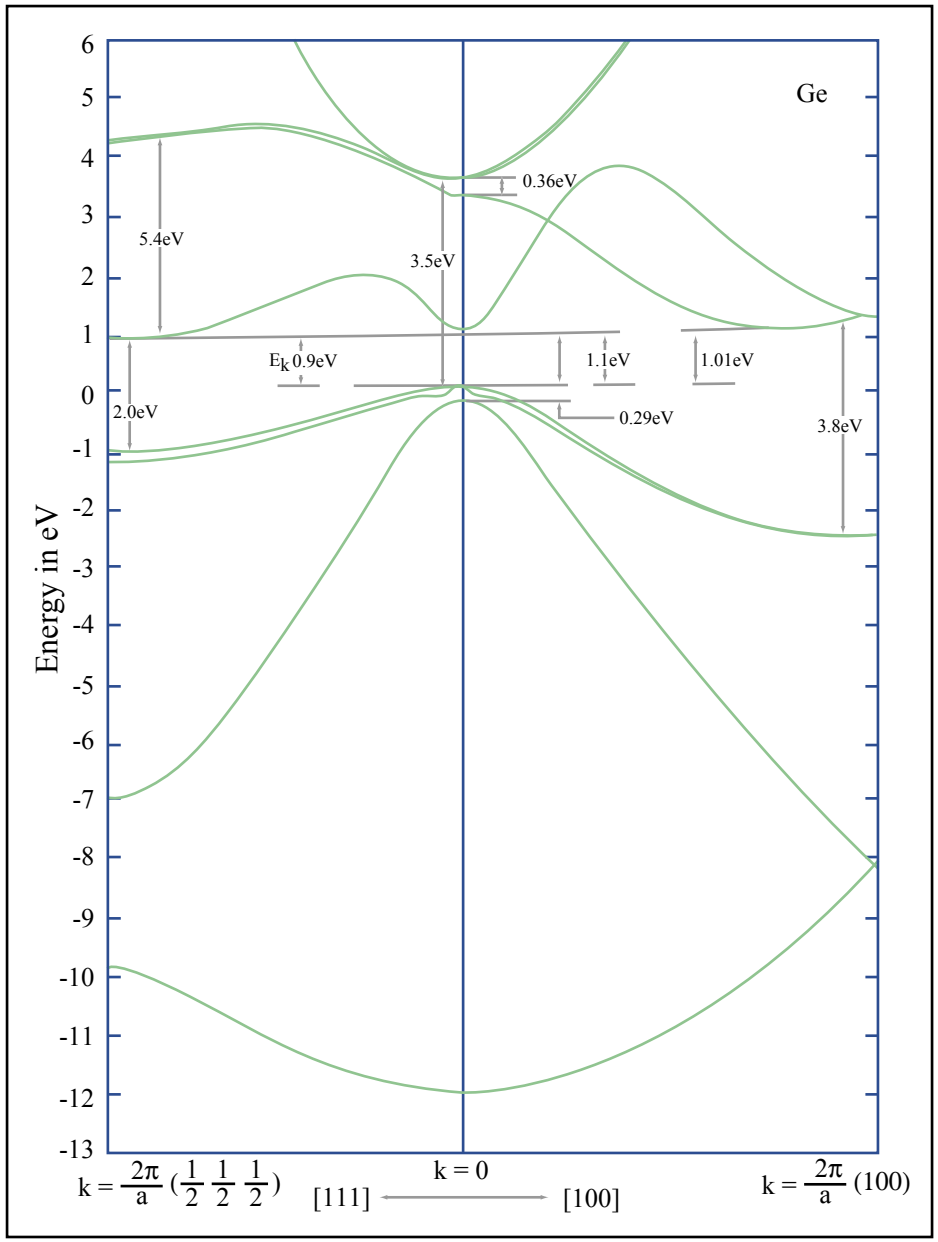


Figure by MIT OpenCourseWare.

Real Band Structures

- Ge: Very close to GaAs, except conduction band minimum is in <111> direction, not at k=0
- Indirect Band Gap



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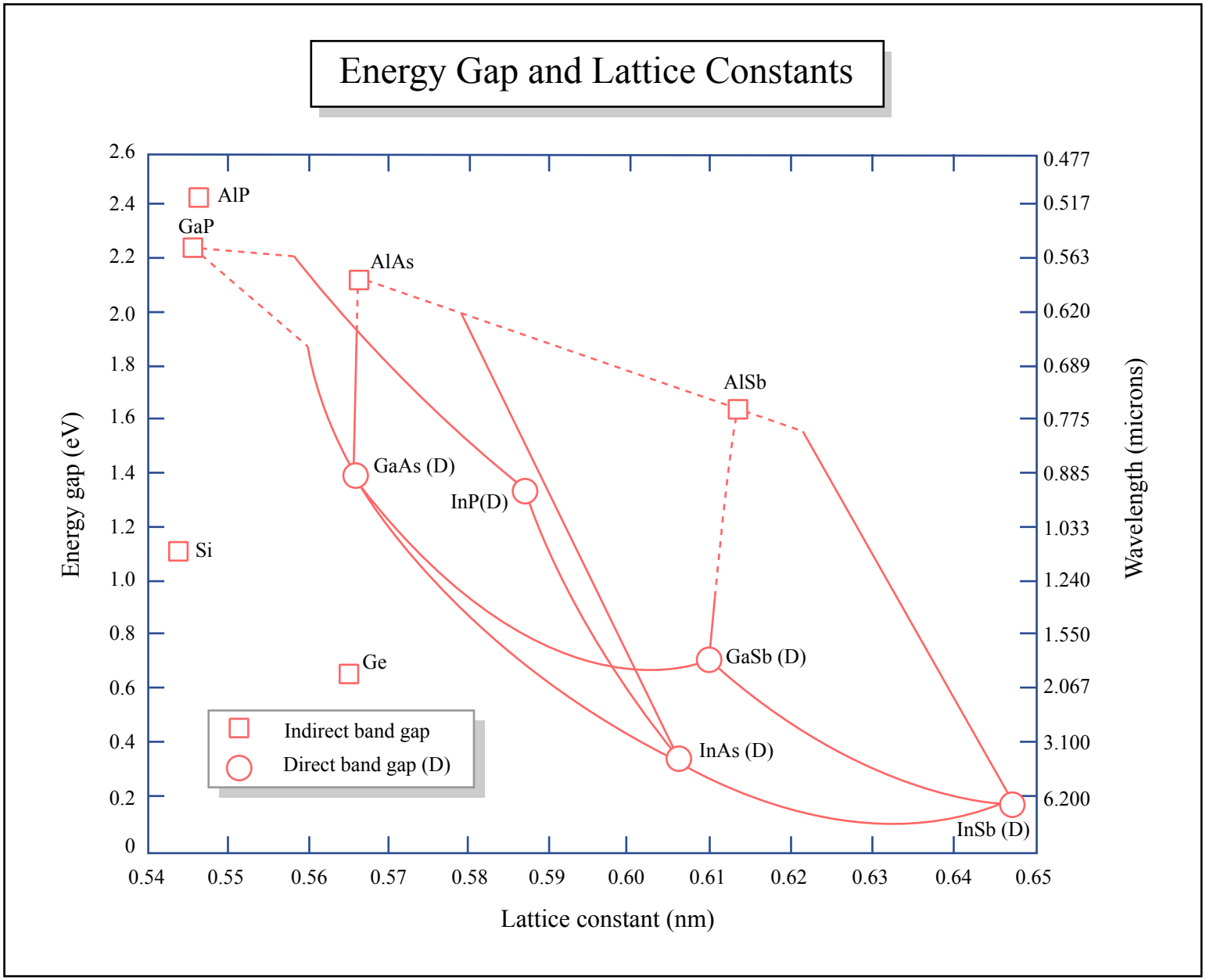
Trends in III-V and II-VI Compounds



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Lattice Constant (A)