

Motivation (Why is this course required?)

- Computers
 - Human based
 - Tube based
 - Solid state based
- Why do we need computers?
 - Modeling
 - Analytical- great for understanding, low accuracy
 - Numerical- high accuracy, impossible to hand calculate

Motivation (Why is this course required?)

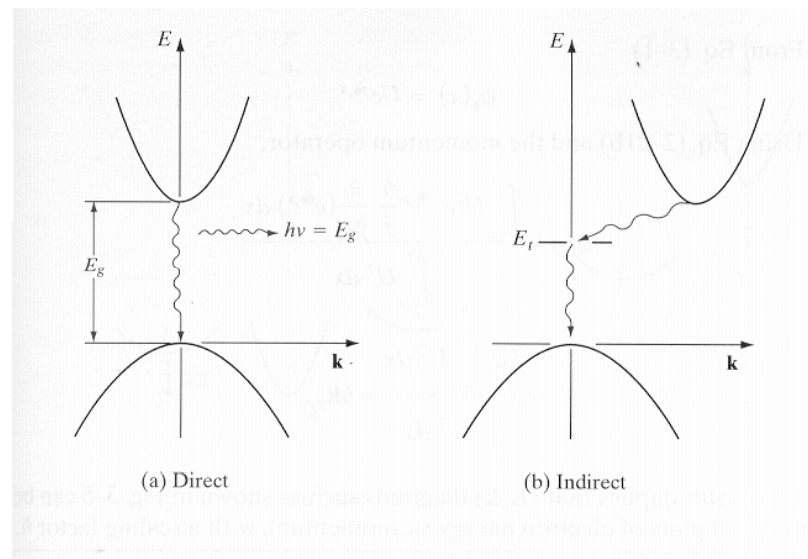
- Analog circuits
 - Human based (?)
 - Tube based
 - Solid state based
- Light emitters/detectors
 - Laser Diodes, LED's
 - Photodiodes
 - Solar Cells

The Bottom line about Energy Bands

- Semiconductors have an energy gap
 - This allows the formation of electrons and holes
 - We want to use Maxwell's equations to describe the drift and diffusion of electrons and holes
 - This is done through the concept of effective mass.
 - The effective mass come from the E-k diagram. The sharper the curve the lower the effective mass

The Bottom line about Energy Bands

- The concept of Energy gap, effective mass, electrons and holes are the basis of all semiconductor devices.



Bonding forces

- Pauli exclusion principle: **No two electrons in an interacting system can have the same quantum numbers.**
 - An **interacting system** is one in which electron wave functions overlap.
 - An electron's **quantum number** describes which **state** it is in.
 - A **state** is a valid place for an electron to occupy.
- We need the Pauli exclusion principle to understand covalent bonding.

Bonding forces

- Covalent
 - Diamond lattice structure (Ge, Si, C)
 - Each atom has 4 neighbors.
 - Each atom shares its electrons with its neighbors.
 - Each bond is composed of two electrons with different spins.
 - Therefore there are no free electrons, thus Si and Ge are insulators at 0K. (What about at higher temperatures?)

Bonding forces

- Covalent/Ionic
 - Zincblende lattice structure (GaAs, InP, ZnSe)
 - Each atom has 4 neighbors that are not of the same type, thus there is ionic bonding
 - Each atom shares some of its electrons with its neighbors, thus there is covalent bonding.
 - The bonding is mixed between ionic and covalent and in general becomes more ionic as you separate across the periodic table(III-V to II-VI).

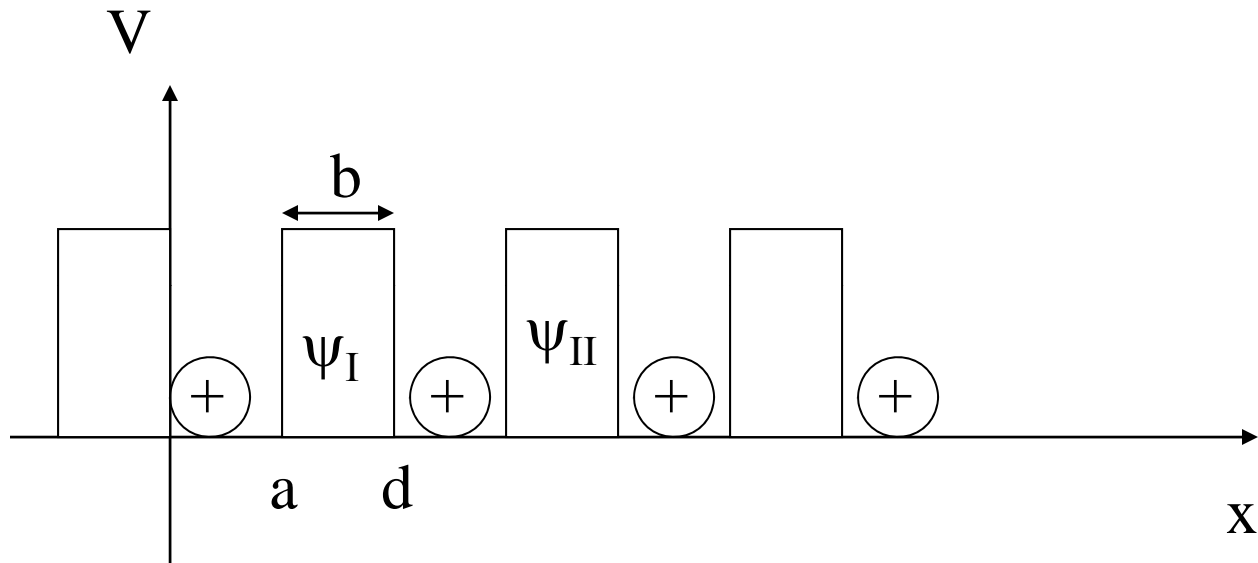
Energy bands

- As atoms are brought closer together their electron wave functions start to interact.
- Two atoms brought close together will see each energy level split into two, three atoms will see a split of three and so on
- A very large amount of atoms will see these discrete levels smear into a band of energy levels.

Energy bands

- These bands of states are separated by forbidden regions.
- The lowest unfilled band is the conduction band (at 0K in semiconductors).
- The highest filled band is the valence band (at 0K in semiconductors).

Energy bands



$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}, (0 \leq x \leq a)$$

$$\frac{\hbar^2 k_1^2}{2m} = E$$

$$\psi_{II}(x) = Ce^{ik_2x} + De^{-ik_2x}, (a \leq x \leq a + b = d)$$

$$\frac{\hbar^2 k_2^2}{2m} = E - V$$

Energy bands

- The function must repeat itself
- The wavefunctions at the boundaries must be equal to each other.
- The derivatives of the wavefunctions at the boundaries must be equal to each other.

Energy bands

- This leads to a system of four equations and four unknowns. If the determinant of this system equals zero then there is a non-trivial solution. After a bit of algebra this leads to the dispersion relation.

Energy bands (Dispersion relation)

$$(E > V)$$

$$\cos k_1 a \cos k_2 b - \frac{k_1^2 + k_2^2}{2k_1 k_2} \sin k_1 a \sin k_2 b = \cos kd$$

$$\frac{\hbar^2 k_1^2}{2m} = E, \frac{\hbar^2 k_2^2}{2m} = E - V$$

$$(E < V)$$

$$\cos k_1 a \cosh \kappa b - \frac{k_1^2 - \kappa^2}{2k_1 \kappa} \sin k_1 a \sinh \kappa b = \cos kd$$

$$\frac{\hbar^2 k_1^2}{2m} = E, \frac{\hbar^2 \kappa^2}{2m} = V - E$$

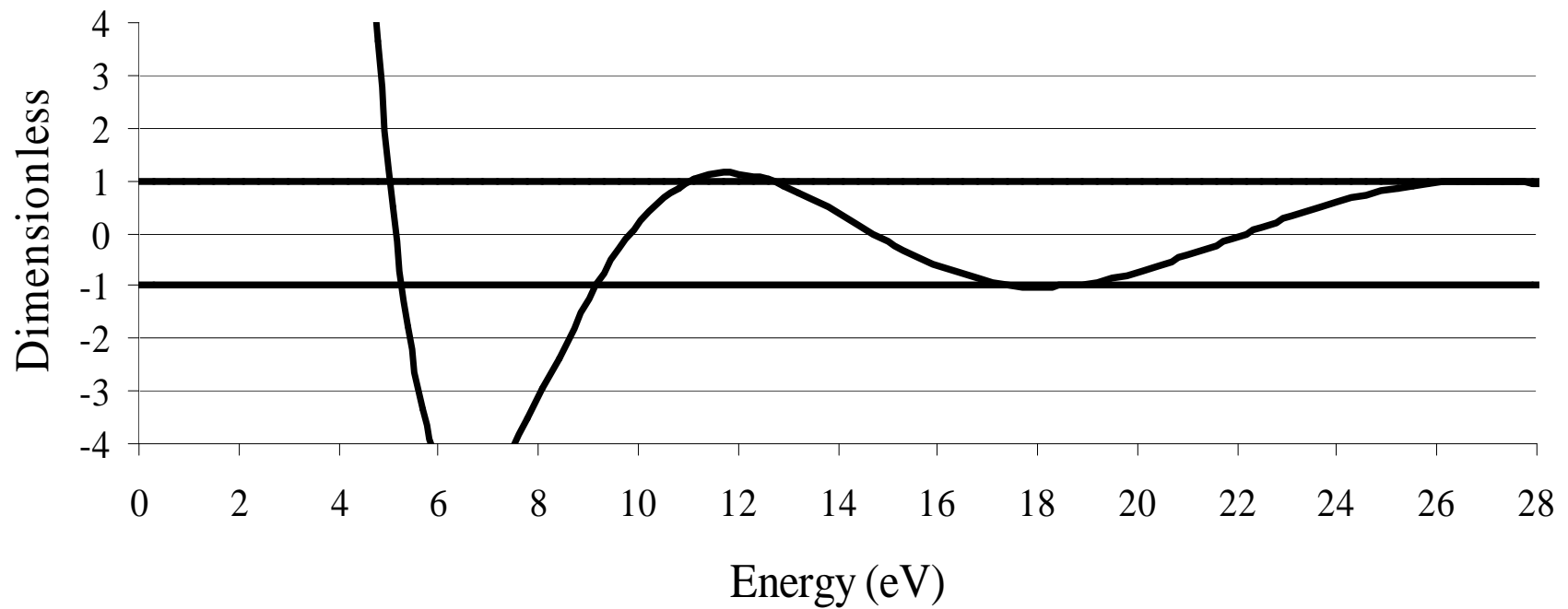
Energy bands

$$d=5.45\text{\AA}$$

$$a=1.1\text{\AA}$$

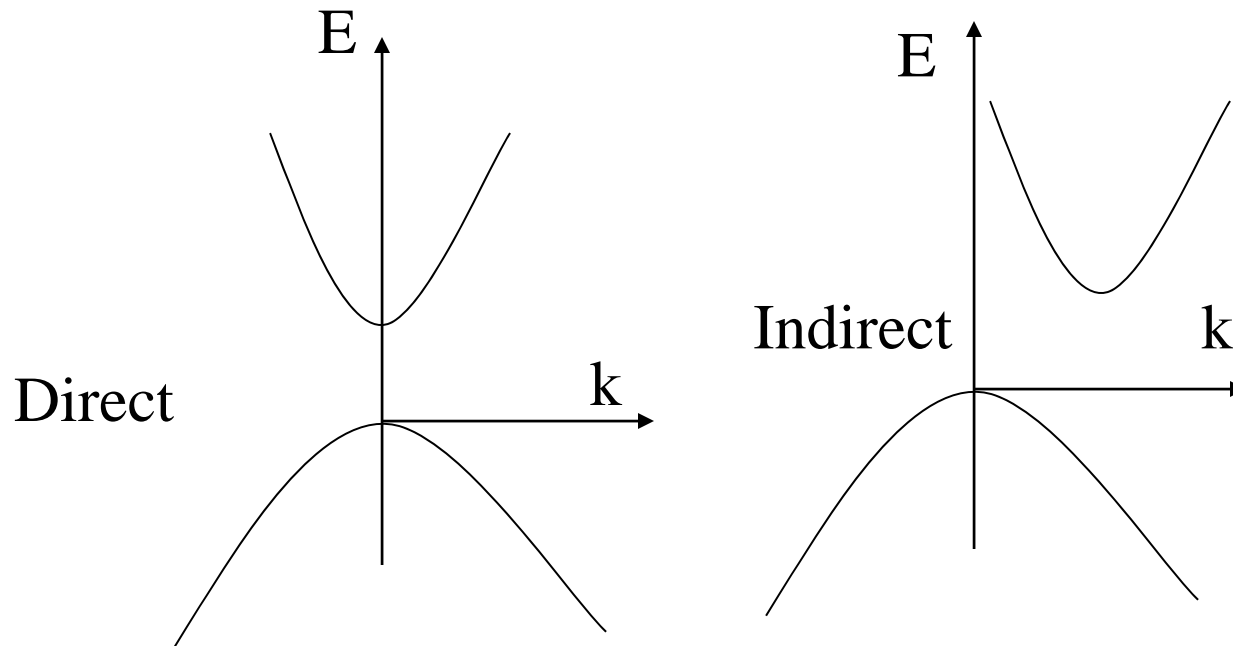
$$V=8\text{eV}$$

Band Structure of the Energy Spectrum of the Kronig-Penny Hamiltonian



Energy Bands

- If you plot the allowed values of energy vs. the propagation constant you get the band structure shown:



Energy Bands

- Insulator (large band gap) hard to move an electron from the valence to the conduction band at any temperature.
- Semiconductor (small band gap optical photons and heat (lattice vibrations) can easily give the required energy to move to the conduction band
- Metals (band gaps overlap), partially filled, easy for current to flow

Energy bands

- The inter-atomic spacing varies with the direction you are moving in the crystal {111} planes would have a smaller d than {100} planes, thus the energy gaps are different in each direction.
- This gives rise to different bands, but usually effect due to this can be averaged.