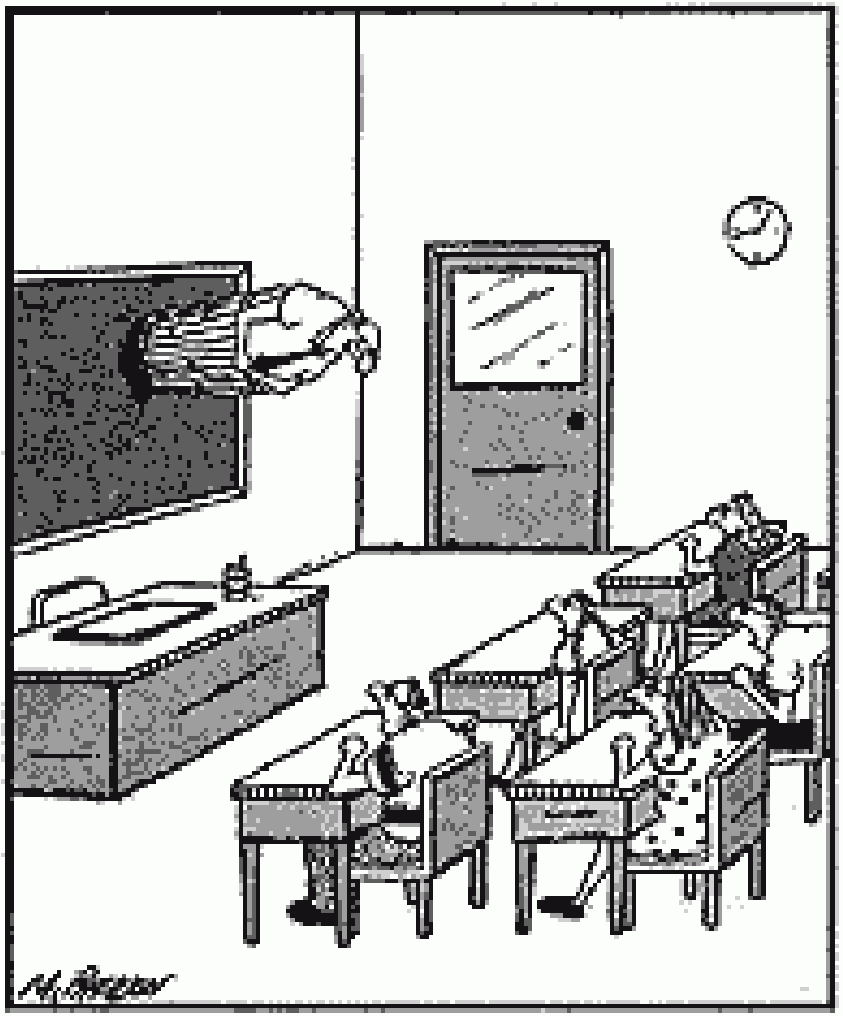
Energy Bands

EECS 320

Introduction to Semiconductor Devices



"Good morning, and welcome to The Wonders of Physics."

Electromagnetics Review

$$\frac{d(\varepsilon F)}{dx} = \rho$$

ε – permittivity of material

***F* – Electric field**

ρ – charge density

$$\varepsilon(F_2 - F_1) = \int_{x_1}^{x_2} \rho(x)dx$$

$$Force = QF$$

$$Force = -qF \text{ (electrons)}$$

$$dW = -qFdx = qdV$$

$$\boxed{F = -\frac{dV}{dx}}$$

Potential Energy

$$P.E. = -qV$$

$$\boxed{F = \frac{1}{q}\frac{dE}{dx}}$$

Poisson's Equation

$$\boxed{\frac{d^2V}{dx^2} = -\frac{\rho}{\varepsilon}}$$

Recall that electrostatic potential, potential energy, etc are *relative to an arbitrary point of reference*

Electromagnetics Review

Poisson's Equation

$$\boxed{\frac{d^2V}{dx^2} = -\frac{\rho}{\varepsilon}}$$

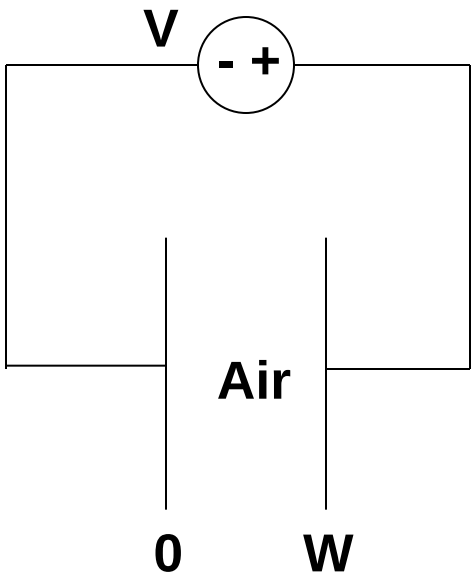
Given charge density,

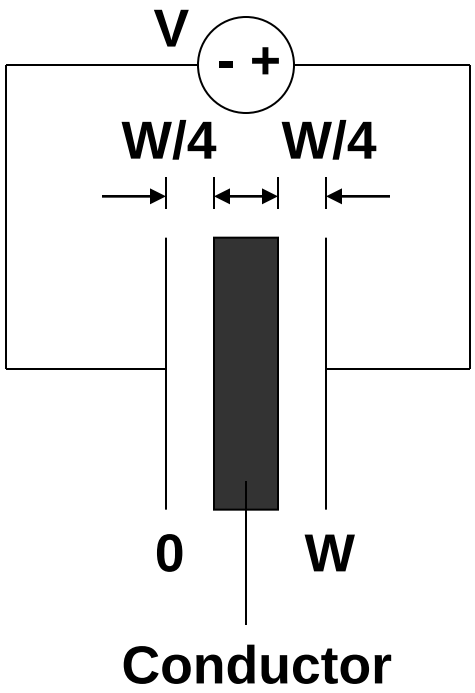
- Integrate once to get electric field
- Integrate twice to get electric potential (and energy)

Electrostatics Examples

Parallel Plate Capacitor

Sketch charge density, field, and electric potential for the following:





Electrons In Solids

How do electrons behave in solids?

Ohm's Law

$$V = IR = AJR$$

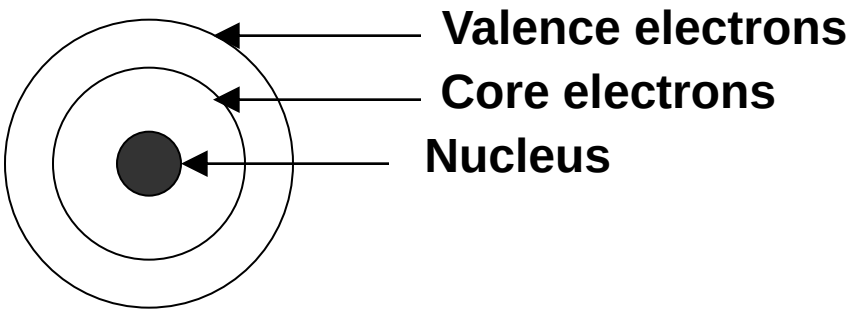
$$R = \frac{\rho L}{A} = \frac{L}{\sigma A}$$

$$J = \sigma F = qnv$$

$$v = \mu F$$

$$\boxed{\sigma = q\mu n}$$

Classical Model



"Free" valence electrons contribute to conductivity

Is this model accurate?

Electrons In Solids

Examine definition of conductivity

$$\boxed{\sigma = q\mu n}$$

Assuming μ is similar for differing materials (proportionality constant for velocity and electric field), compare σ for Al, C

$$n = 6.02\times10^{23}\,\frac{(\#elec/atom)(\text{density in } g/\text{cm}^3)}{\text{Atomic mass in } g/\text{mol}}\left(cm^{-3}\right)$$

<u>Aluminum</u>

3 valence electrons

$$density = 2.7\,g/\text{cm}^3$$

$$\text{Atomic mass} = 27\,g/mol$$

$$n = 1.8\times10^{23}cm^{-3}$$

<u>Carbon</u>

4 valence electrons

$$density = 3.52\,g/\text{cm}^3$$

$$\text{Atomic mass} = 12\,g/mol$$

$$n = 7.1\times10^{23}cm^{-3}$$

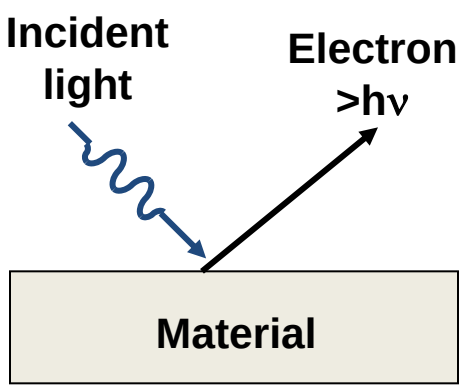
Does this make sense?

Principles Of Quantum Mechanics

Energy Quanta

Emitted radiation takes on discrete energies

Photoelectric Effect



Ejection depends on E, not intensity

Wave-Particle Duality

Waves show particle-like behavior (photon-light)

Particles show wave-like behavior (electron-wave)

de Broglie Wavelength

$$\lambda = \frac{h}{p}$$

Uncertainty Principle

Uncertainty in position/momentum of particle and energy/momentum of wave

$$\Delta p \Delta x \geq \hbar$$

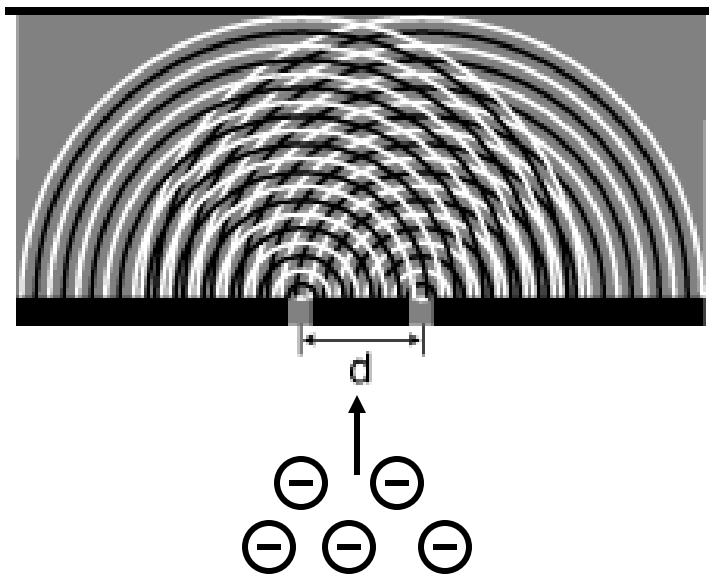
$$\Delta E \Delta t \geq \hbar$$

Describe using probability

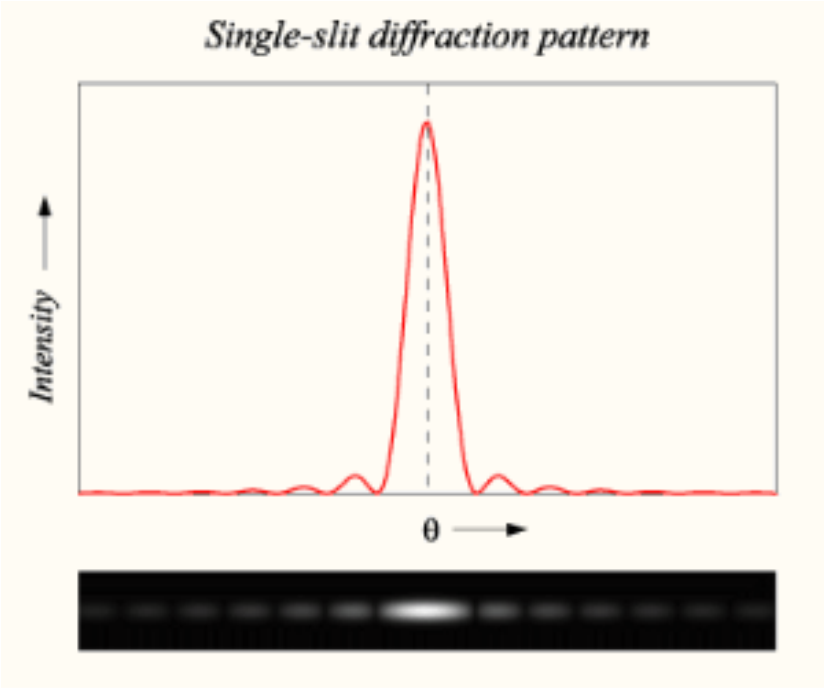
Double-Slit Experiment

Electron beam incident on "double-slit"
Detect electrons on other side

detect here



Result



Electrons have wave-like properties

Electromagnetic Wave Equation in Free Space

Maxwell's Eqn's in Free Space

$$\nabla \bullet \vec{E} = 0$$

$$\nabla \bullet \vec{B} = 0$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{B} = \mu_0 \varepsilon_0 \frac{\partial \vec{E}}{\partial t}$$

$$\nabla \times \left(\nabla \times \vec{E}\right) = \left\{\nabla\left(\nabla \bullet \vec{E}\right) - \nabla^2 \vec{E}\right\} = \nabla \times \left(-\frac{\partial \vec{B}}{\partial t}\right) = -\frac{\partial}{\partial t}\left(\nabla \times \vec{B}\right)$$

$$-\nabla^2 \vec{E} = -\frac{\partial}{\partial t}\left(\nabla \times \vec{B}\right) = -\frac{\partial}{\partial t}\left(\mu_0 \varepsilon_0 \frac{\partial \vec{E}}{\partial t}\right)$$

$$\nabla^2 \vec{E} = \mu_0 \varepsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2}$$

$$\left(\nabla^2 - \mu_0 \varepsilon_0 \frac{\partial^2}{\partial t^2}\right)\vec{E} = 0$$

similarly

$$\left(\nabla^2 - \mu_0 \varepsilon_0 \frac{\partial^2}{\partial t^2}\right)\vec{B} = 0$$

$$c = \frac{1}{\sqrt{\mu_0 \varepsilon_0}}$$

Wave Propagation In Free Space

$$\left(\nabla^2 - \mu_0 \varepsilon_0 \frac{\partial^2}{\partial t^2}\right)\vec{E} = 0$$

$$\vec{E} = E_x e^{i(kz-\omega t)}\hat{z} \quad \text{Plane Wave}$$

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

$$\omega = 2\pi\nu$$

EM Wave in a box

- Perfectly conducting walls

Rationalization of Schrödinger's Equation

- Lots of Evidence of Wave-like Behavior of Electrons
- As soon as we have wave phenomenon:
  - Look for Wave Equation(s) (aka. Maxwell, Acoustics)
- Natural Thing to do is to consider plane wave (sinusoidal) solutions

$$\lambda = \frac{h}{p}$$ Observed from Electron Diffraction

$$p = \frac{h}{\lambda} = \frac{hk}{2\pi} = \hbar k$$ DeBroglie's Hypothesis

For a plane wave

$$\psi\left(\vec{r}\right) = Ae^{i\left(\vec{k}\bullet\vec{r}-\omega t\right)}$$

We have

$$\nabla^2\psi = -k^2\psi$$

or

$$-\hbar^2\nabla^2\psi = +\hbar^2k^2\psi = p^2\psi$$

$$KE = \frac{1}{2}mv^2 = \frac{\left(mv\right)^2}{2m} = \frac{p^2}{2m}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \left(KE\right)\psi$$

$$Total\ \ Energy = KE + PE = E$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + U\right)\psi = E\psi$$ Schrodinger's Wave Equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + U\right)\psi = \left(i\hbar\frac{\partial}{\partial t}\right)\psi$$

Electron States In A Hydrogen Atom

Solution Of Schrodinger's Equation Results In Quantized Electron States

Schrodinger's Equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi = E\psi$$

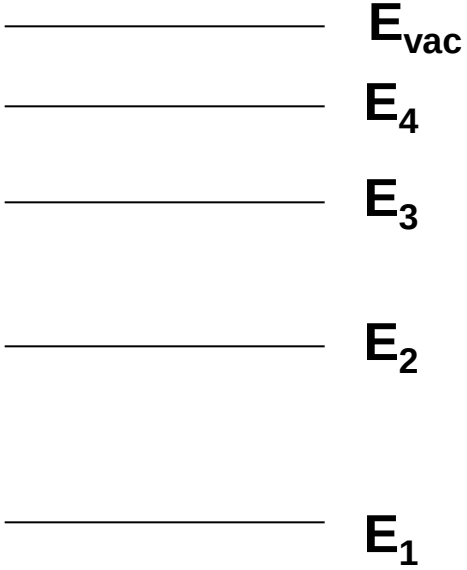
$$i\hbar\frac{\partial\psi}{\partial t} = E\psi$$

Solution

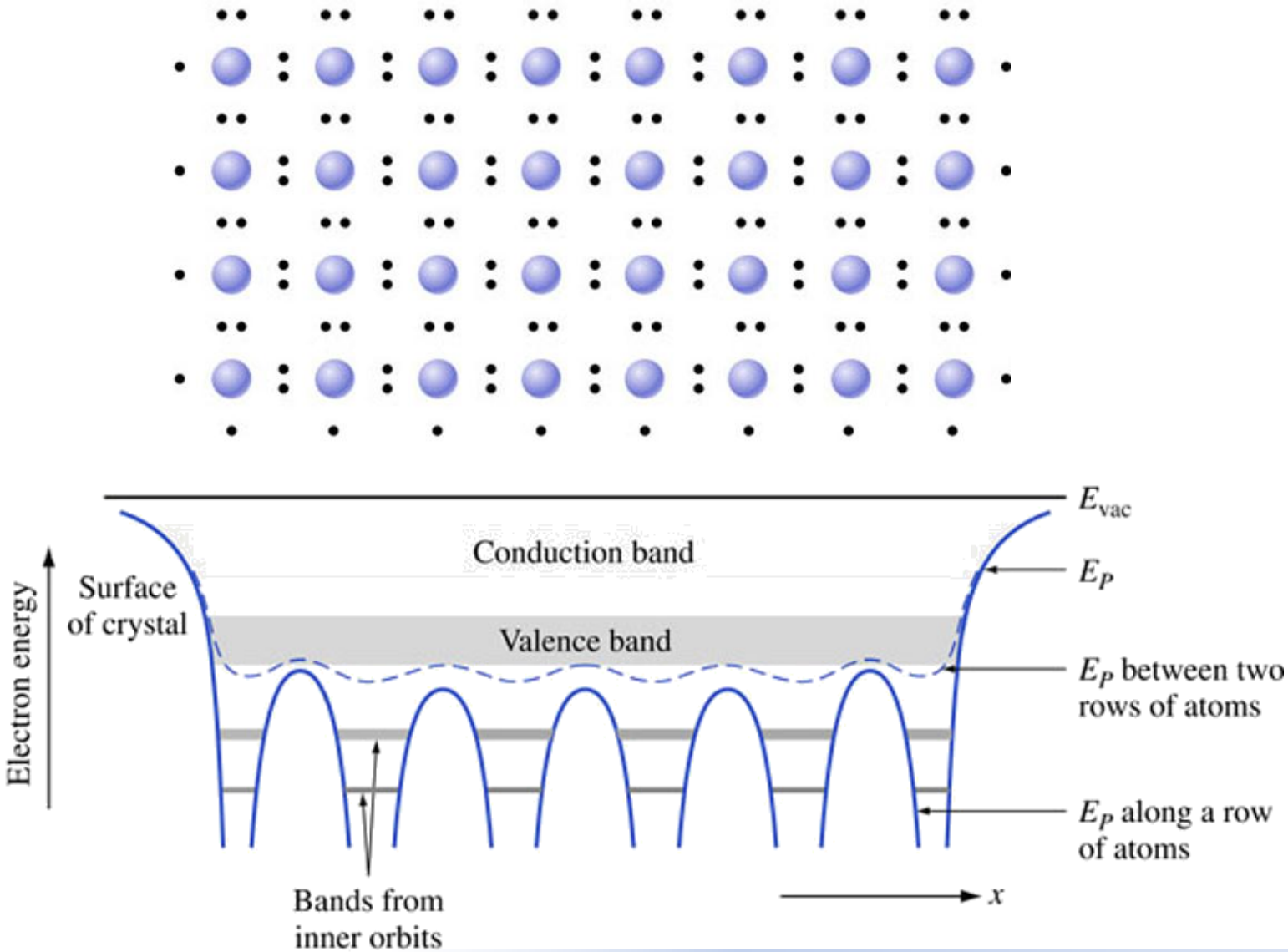
$$E = -\frac{m_0 q^4}{2\left(4\pi\varepsilon_0\hbar \mathrm{n}\right)^2} = -\frac{13.6}{\mathrm{n}^2}eV$$

$$\mathrm{n} = 1,2,3,\ldots$$

Discrete Energy Levels

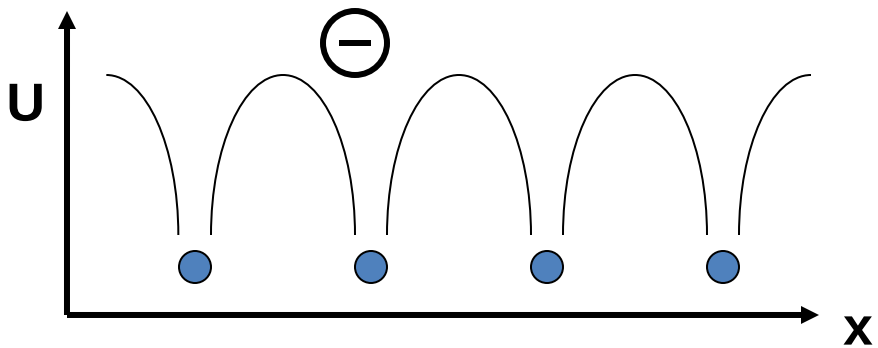


Covalent Bonding in a Crystal



Electronic Potential in a Crystal

The potential in a semiconductor varies on the order of the DeBroglie wavelength of an electron



$$\lambda = \frac{h}{p}$$

Quantum Mechanics must be used to describe electronic properties

Schrodinger's Equation

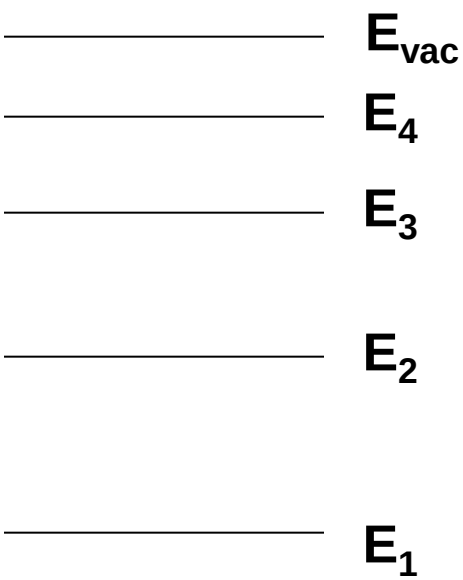
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi = E\psi$$

$$i\hbar\frac{\partial\psi}{\partial t} = E\psi$$

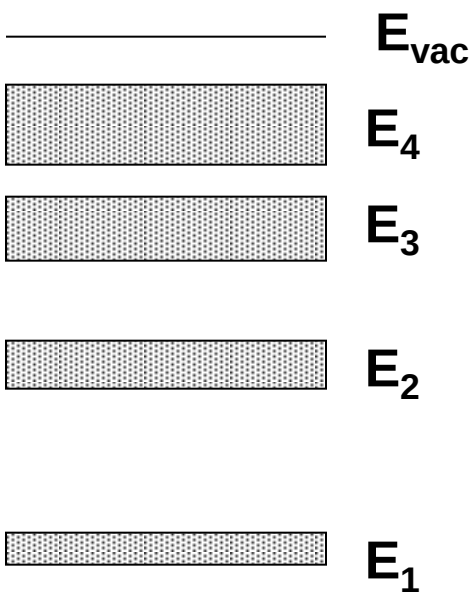
Electronic States in a Crystal

Schrodinger's equation may be solved in a semiconductor due to the periodic potential

Atom:
Discrete Energy Levels



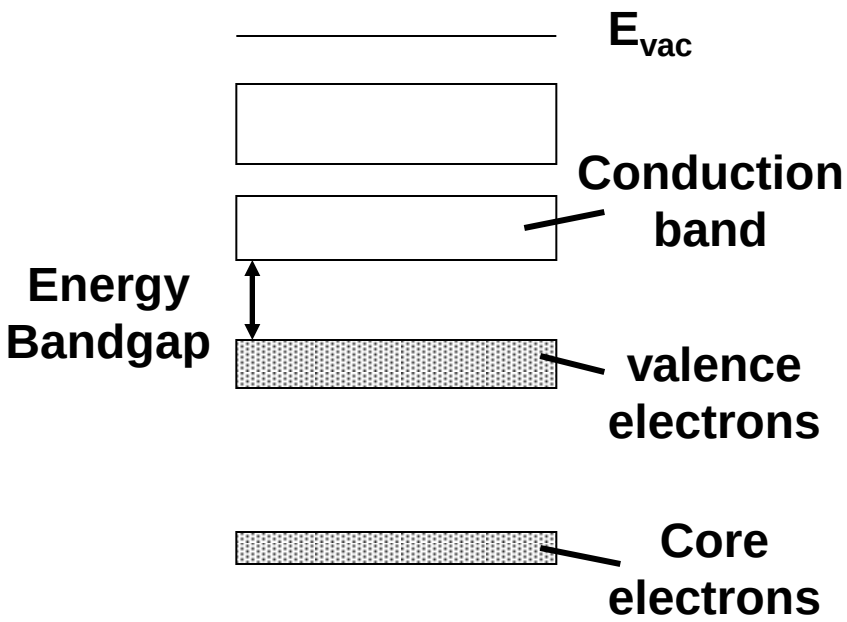
Semiconductor:
Energy Bands



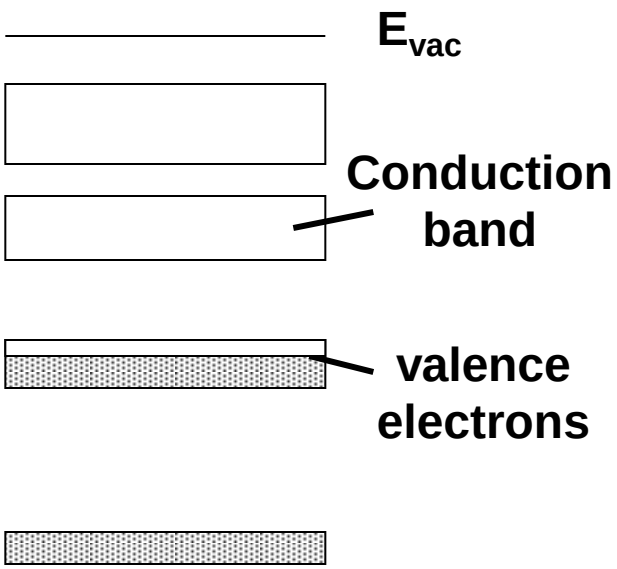
Conduction and Valence Bands

Valence electrons define conductivity

Semiconductor
Valence band filled with electrons



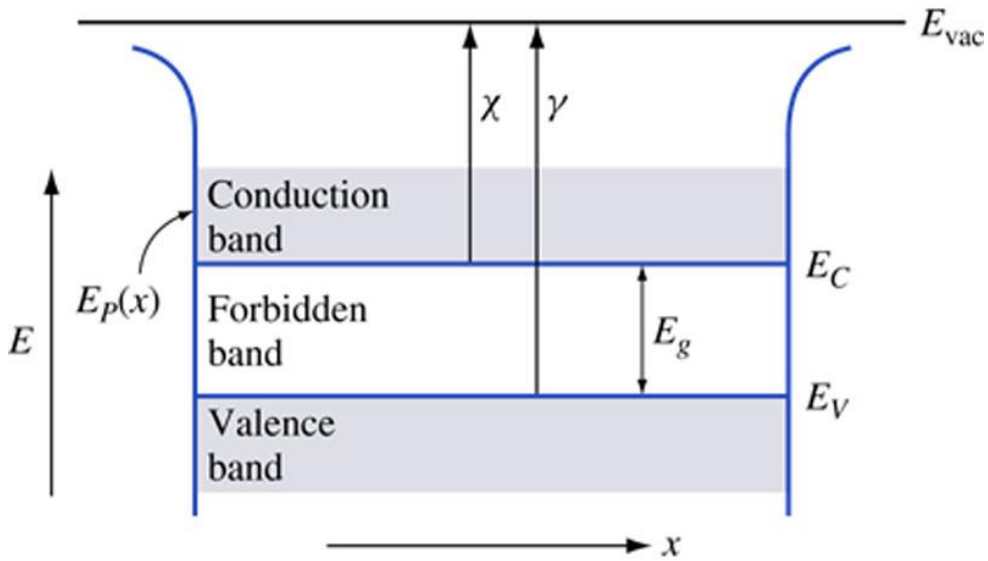
Metal
Valence partially filled with electrons

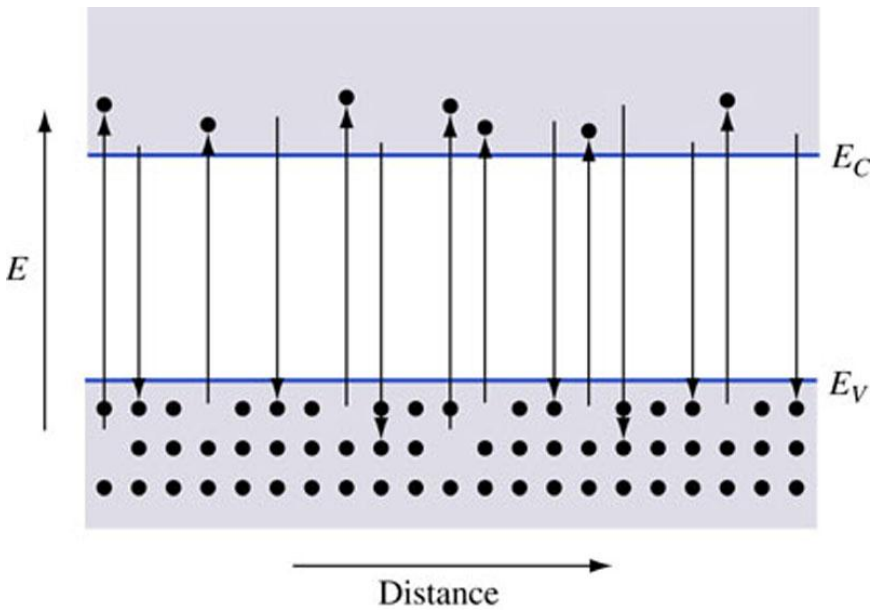


Energy Bands

Definitions

- **Electron affinity (χ)**
- **Bandgap energy (E_g)**





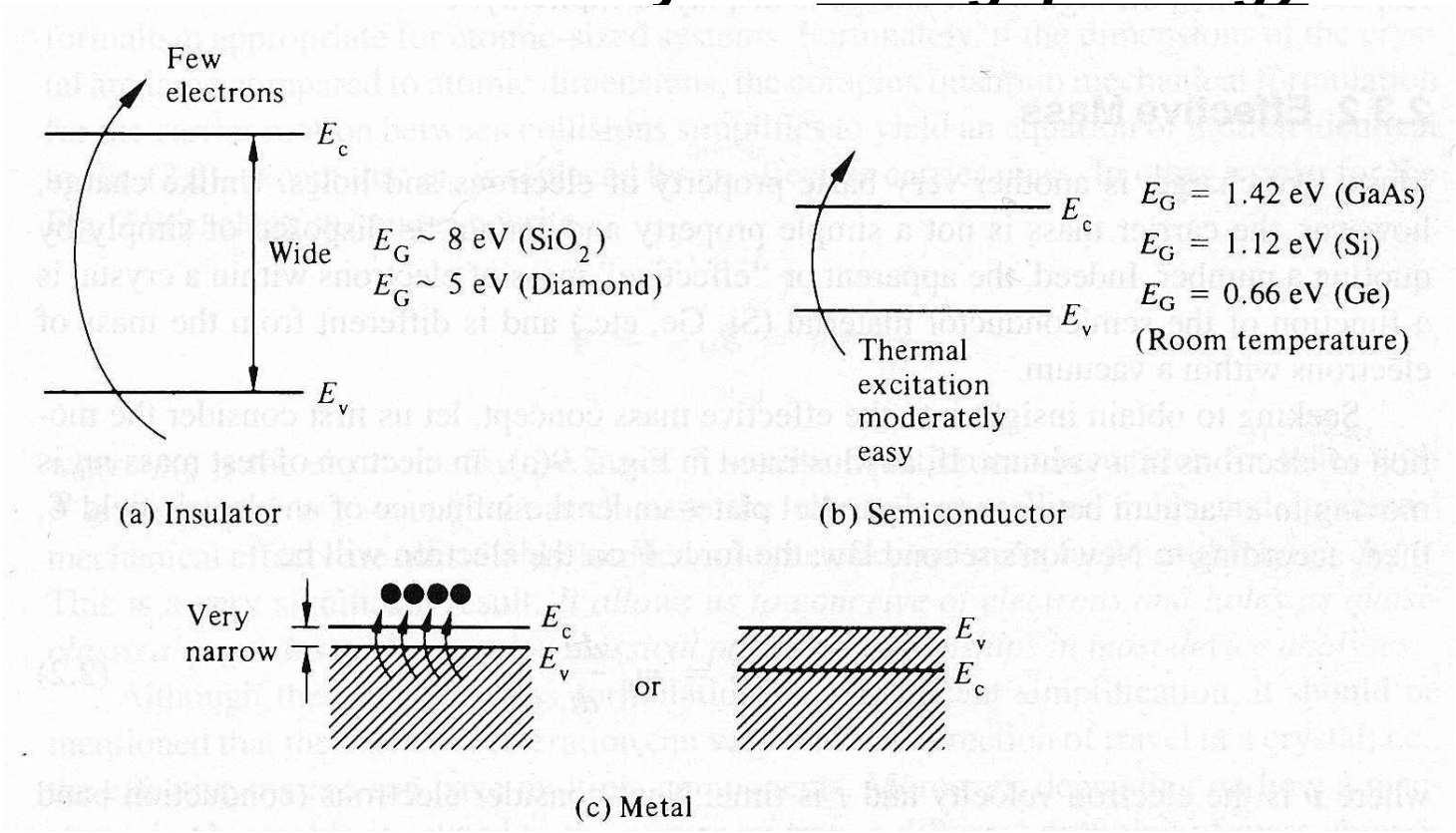
Which electrons contribute to conduction?

Energy Band Diagrams

How do you distinguish between a metal, semiconductor, and an insulator?

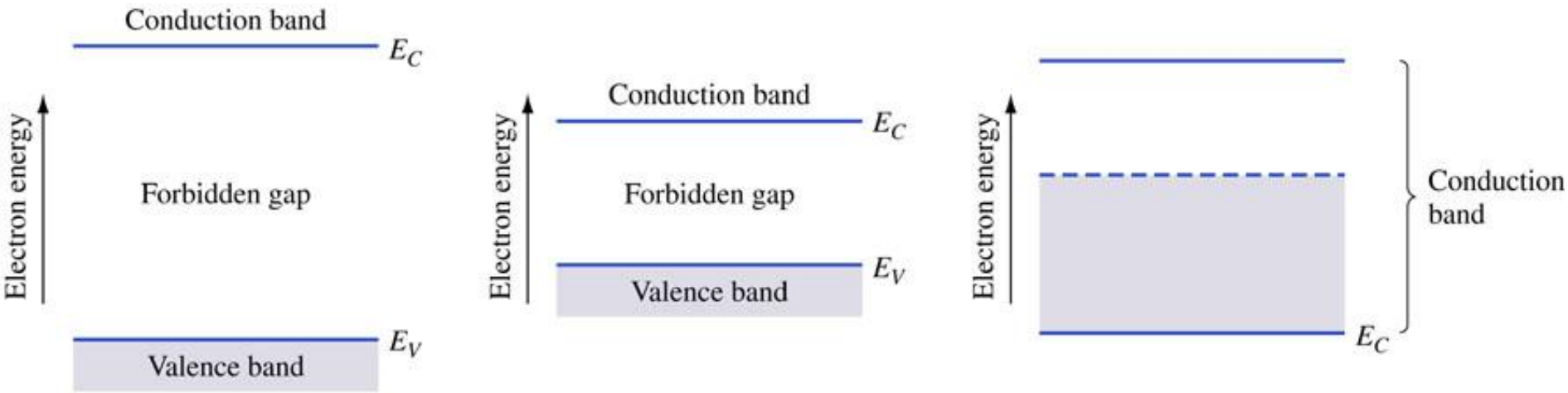
Bandgap Energy

Many of the electronic properties of a material will be determined by the *bandgap energy*



Bandgap energy is a *material parameter*

Conductors, Semiconductors, and Insulators



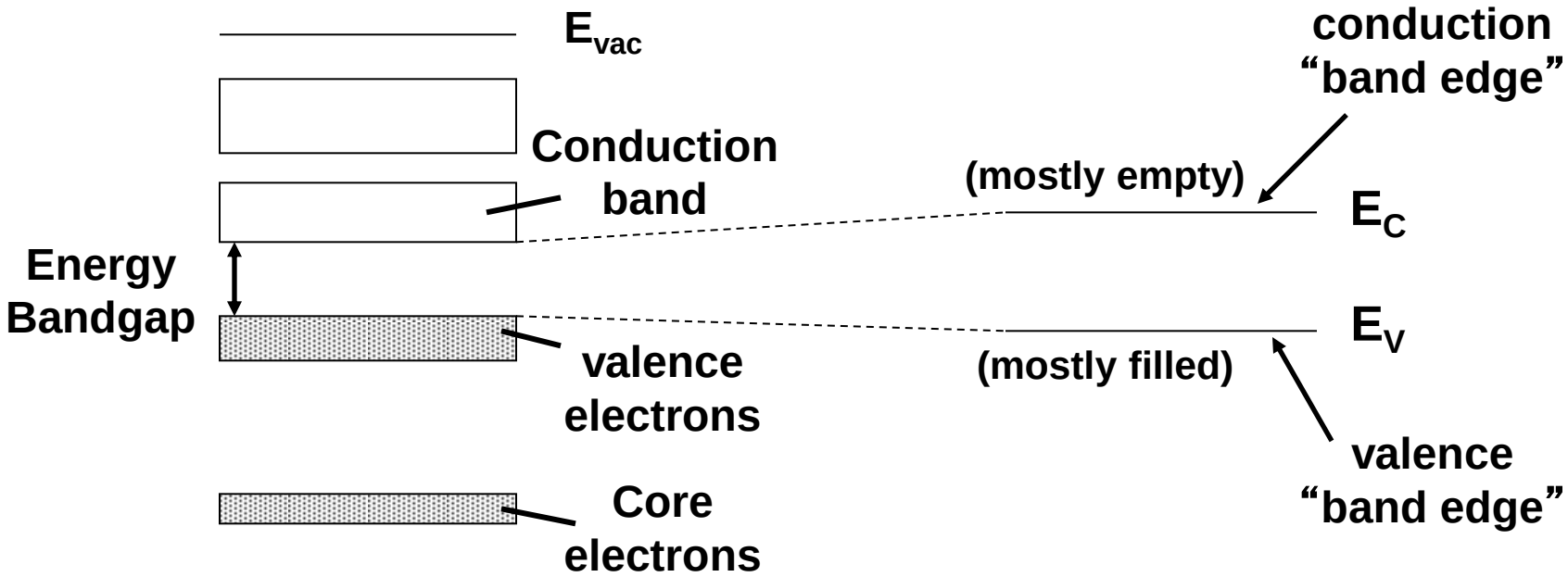
(*a*) Insulator (*b*) Semiconductor (*c*) Metal

What If:

- **Bandgap energy is small?**
- **High temperature?**
- **Low temperature?**

Energy Band Diagram

Primarily concerned with edge of conduction and valence bands



"If you can't draw the energy band diagram, you don't know what you are talking about"

- Herbert Kroemer 2000
Nobel Physics Laureate

Electrons In A Crystal

Free electrons in a vacuum respond to applied electric fields by the following

$$\text{Force} = -qF = m_0 \frac{dv}{dt}$$

("-" sign for electron)

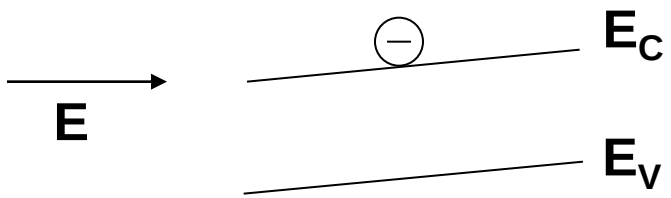
m_0=electron rest mass

q=charge on an electron (1.6×10^{-19} C)

F=electric field

v=velocity

Do electrons in the conduction band of a crystal follow the same relationship?



Wavevector "k"

From de Broglie

$$p = \frac{h}{\lambda}$$

p=momentum **λ=wavelength**

h=Planck's constant (6.63x10^{-34} J-s)

A convenient description of momentum is the wavevector

$$k = \frac{2\pi}{\lambda} \longrightarrow p = \hbar k \qquad \hbar = \frac{h}{2\pi} = 1.06 \times 10^{-34} J - s$$

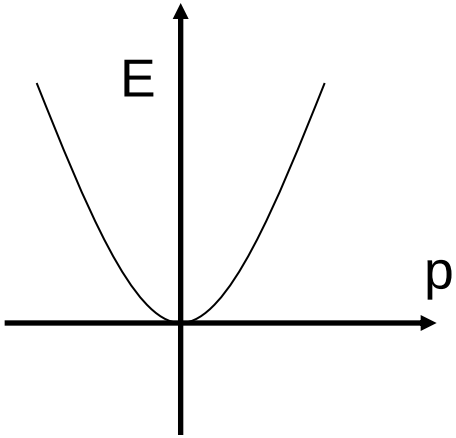
Relation to force and energy

$$\text{Force} = m_0 \frac{dv}{dt} = \frac{dp}{dt} = \hbar \frac{dk}{dt} \qquad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

(Kinetic energy)

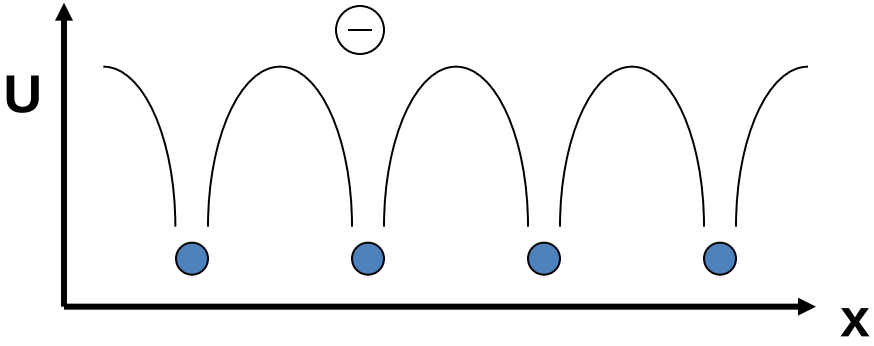
Electrons In A Crystal

Free electron energy-momentum relationship



$$E = \frac{p^2}{2m_0}$$

Electron sees potential variation in crystal



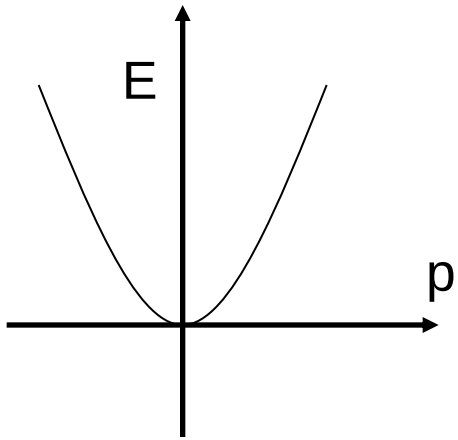
Does E vs p look the same as for free electron?

Effective Mass

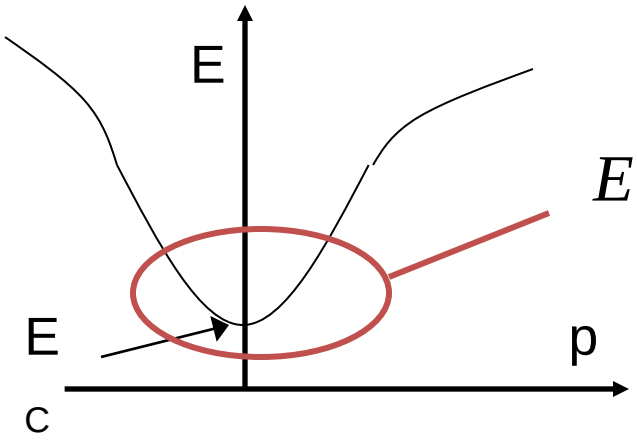
Energy-Momentum Relations In A Semiconductor

- Complex relationship described by quantum mechanics, commonly referred to as the "bandstructure"
- Near E_C, approximately parabolic
- Replace m_0 with m_n^* - *effective mass*

Free electron



Semiconductor



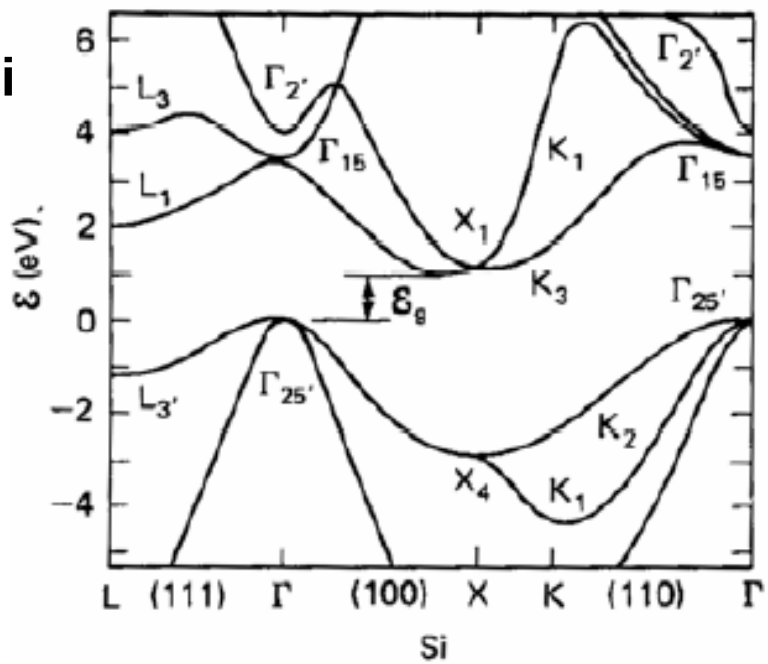
$$E \approx \frac{p^2}{2m_n^*}$$

$$p = \hbar k$$

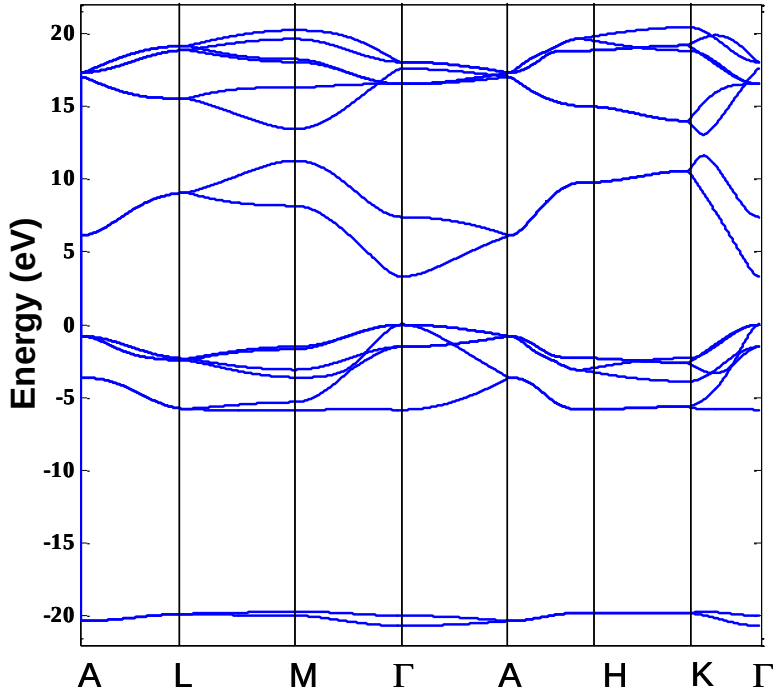
Energy-Momentum Relation (Bandstructure)

E vs k is really "4-D", we typically plot E vs. k in two-dimensions for a particular k direction

Si



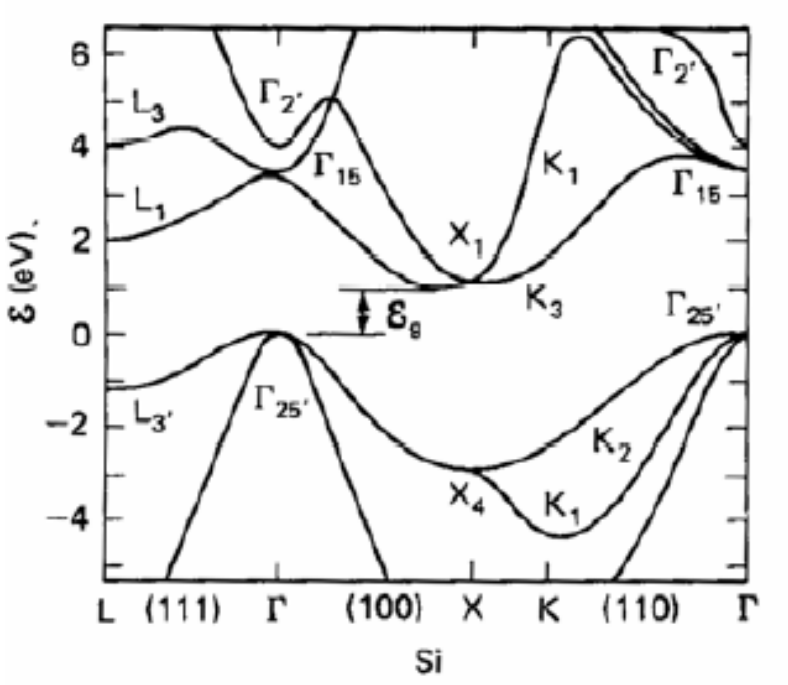
ZnO



- Bandstructure informs us of physical properties
- Typically only interested in small region near conduction and valence band edge
- In this course, we will rarely refer to E vs k, but rather use results in form of constants E_G, m^*, etc.

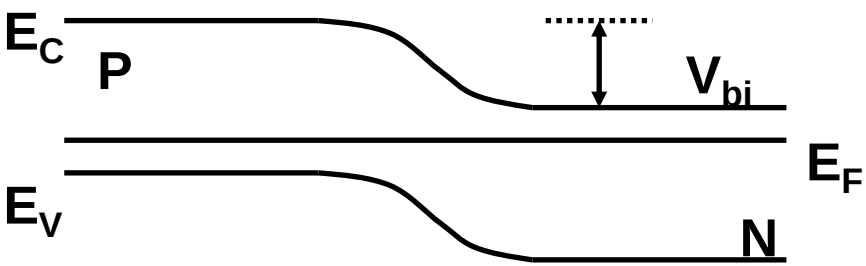
"Real space" versus "momentum-space"

E vs. k (Bandstructure)



- Physical properties
- E_G, m^*,direct vs indirect, etc

Real space (Band diagram)



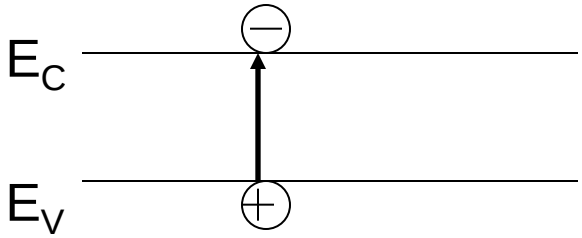
- Device operation
- No distinction between m^*, etc

We will often refer to E vs x ("band diagram") in this course

Charge Carriers In Semiconductors

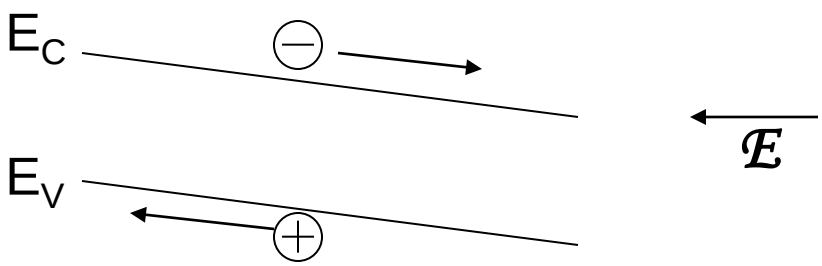
What happens when a valence electron is excited into the conduction band?

- An empty electron state is left behind in the valence band
- Electrons in the valence band fill the empty state, current flow is allowed
- The empty state appears to respond as if it has a positive charge
- We will call the empty state a "hole", and consider the hole to be a positively charged particle



Charge Carriers In Semiconductors

Electrons in the conduction band and holes in the valence band both conduct current

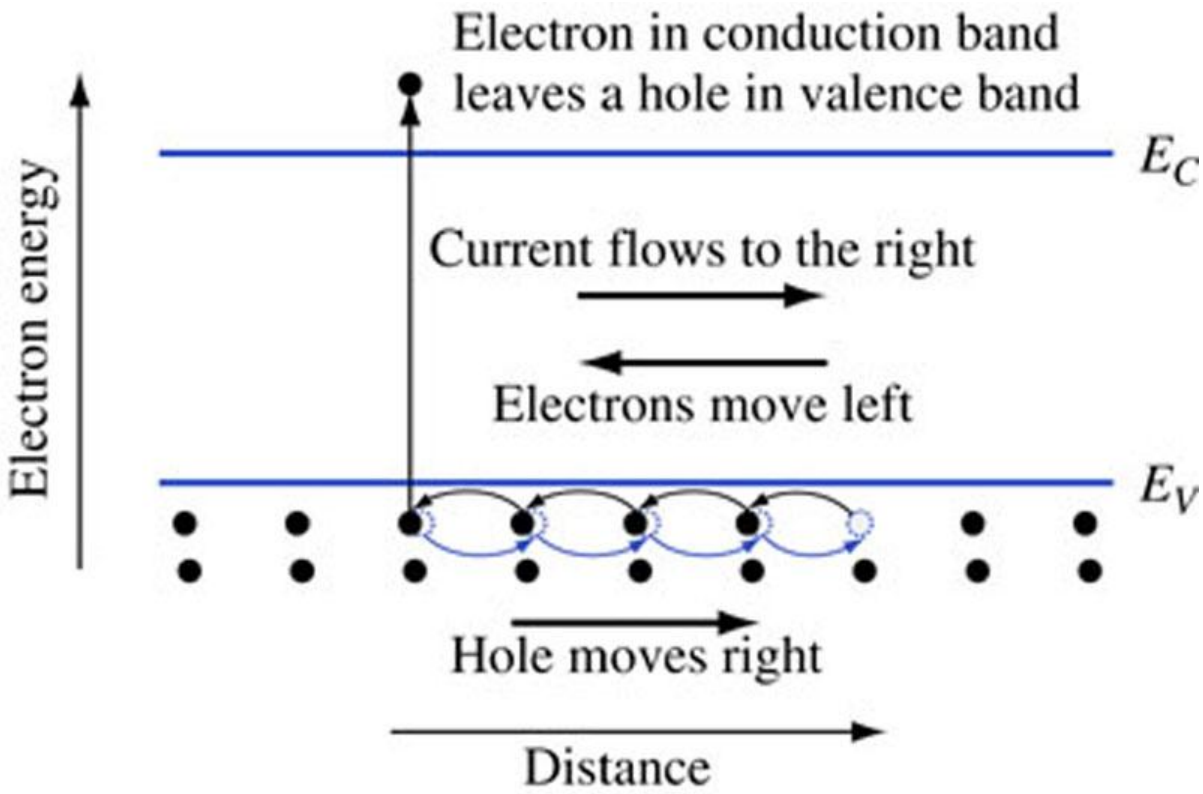


Electrons: like ball rolling down hill

Holes: like bubble floating to surface

Two *independent* conduction mechanisms

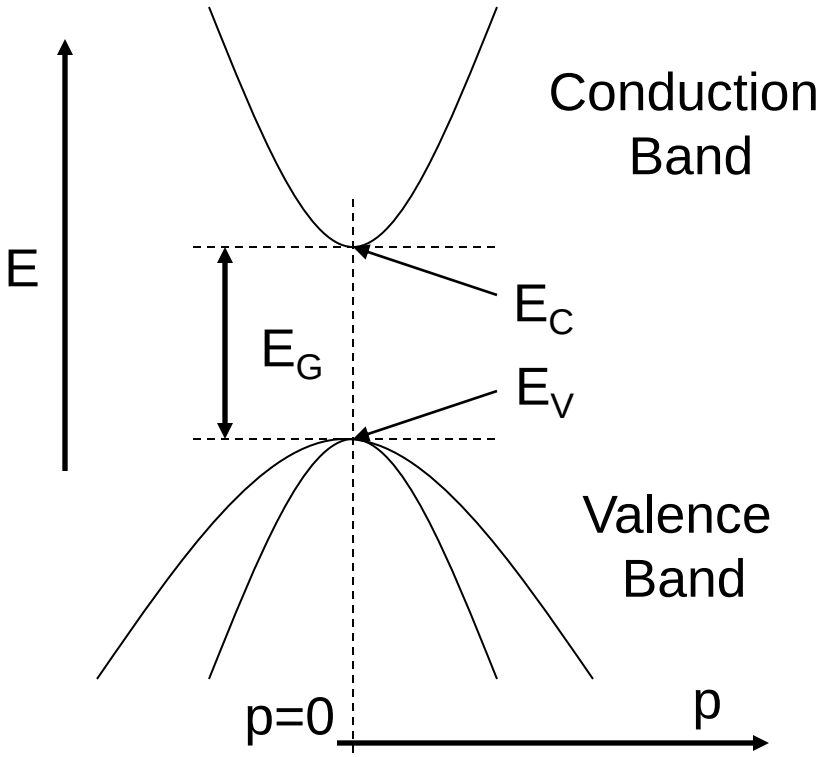
Electrons and Holes



Charge conduction can occur in both the conduction *and* the valence band

Effective mass for holes

Effective mass defined similarly for holes

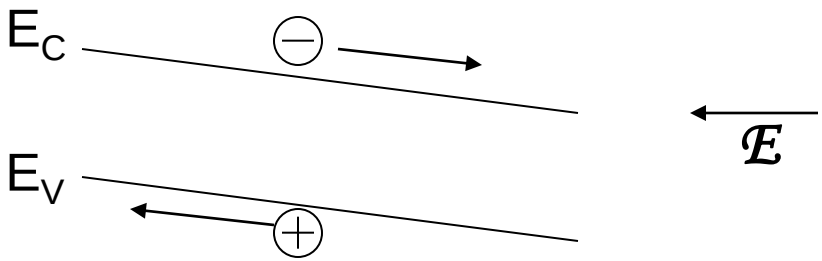


- There is typically a degeneracy at E_V
- Degeneracy results in "light hole" and "heavy hole"
- Define m_h* for given semiconductor, includes light/heavy holes

Electronic Properties Of Semiconductors

Now we have a basic idea of energy bands in a material

To determine electronic properties, we need to answer the following questions



- What is "n" the number of electrons (or "p", number of holes) able to provide current flow?
- What is the number of available electron (hole) states in a semiconductor?
- How are charge carriers distributed in energy?
- Can we alter the number of charge carriers in a material?