

3-D Crystal Structure

- **General**: A crystal structure is defined by **primitive lattice vectors** $\vec{a}_1, \vec{a}_2, \vec{a}_3$.
 - $\vec{a}_1, \vec{a}_2, \vec{a}_3$: Depend on geometry. Once specified, the **primitive lattice structure** is specified.
 - Generate lattice by translating through a **direct lattice vector**: $\vec{r} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$. (n_1, n_2, n_3) are integers. \vec{r} generates the lattice points. Each lattice point corresponds to a set of (n_1, n_2, n_3).
- (3d vectors)**: Have arrows over them. Where it's obvious from context of discussion, may leave this off.)

- Basis (or basis set) \equiv

The set of atoms which, when placed at each lattice point, generates the crystal structure.

- Crystal Structure \equiv *Primitive lattice structure + basis*. Translate the basis through all possible lattice vectors $\vec{r} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$ to get crystal structure or the

DIRECT LATTICE

Diamond & Zincblende Structures

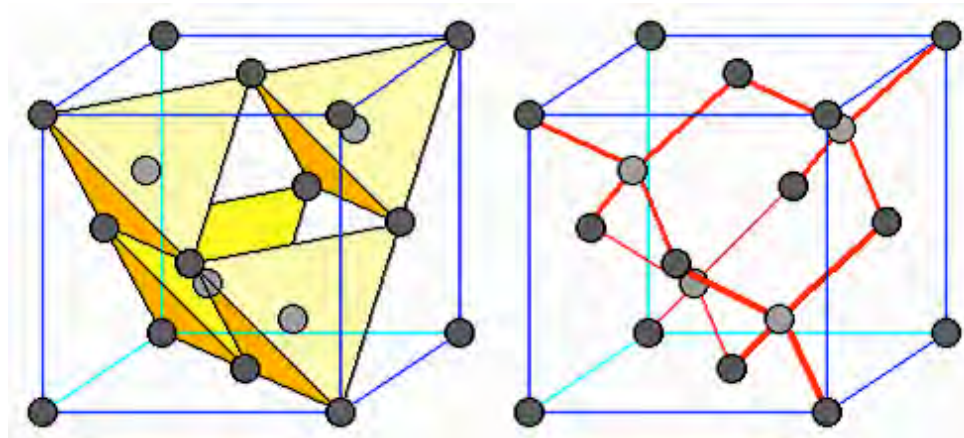
Tetrahedral coordination: Each atom has 4 nearest-neighbors (nn).

Basis set: 2 atoms. **Primitive lattice** \equiv face centered cubic (fcc).

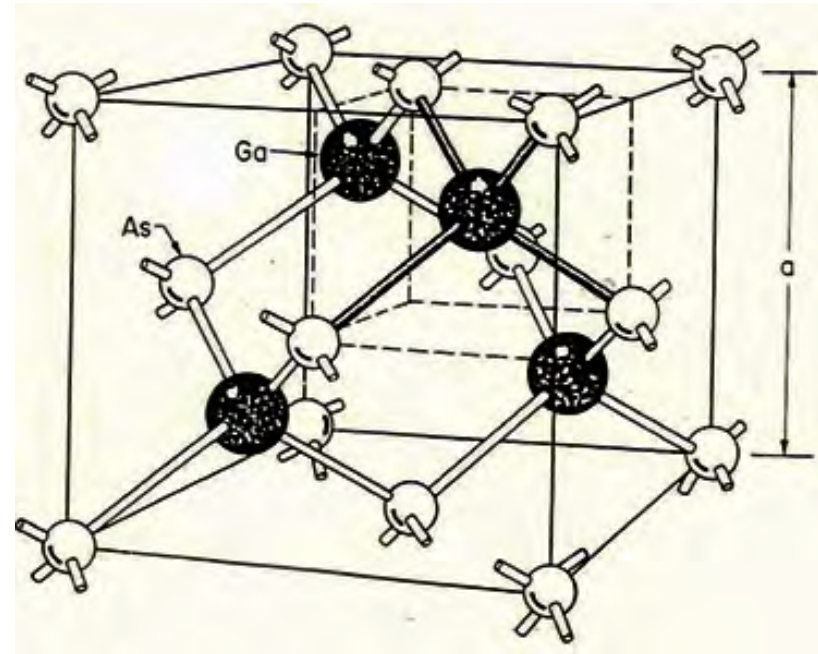
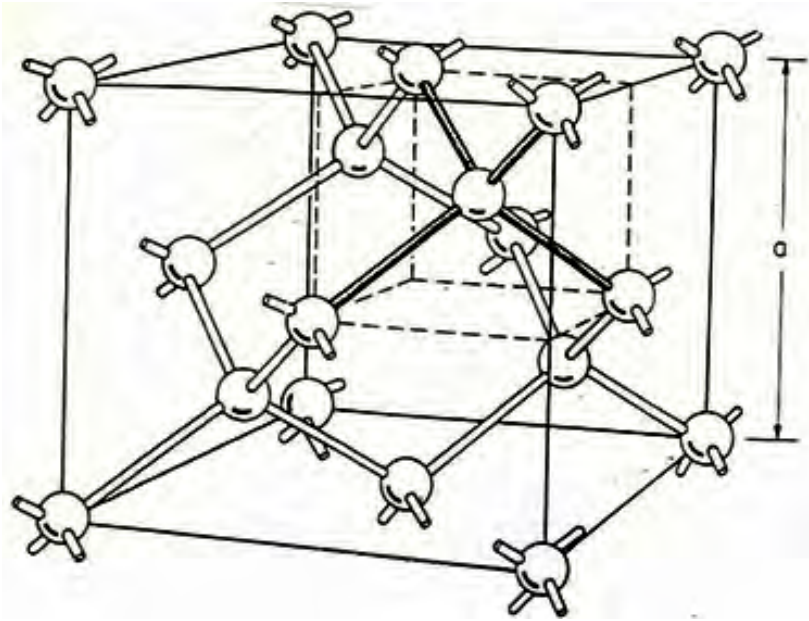
Diamond or Zincblende \equiv 2 atoms per fcc lattice point.

Diamond: 2 atoms are the same. ***Zincblende:*** 2 atoms are different.

Cubic Unit Cell looks like

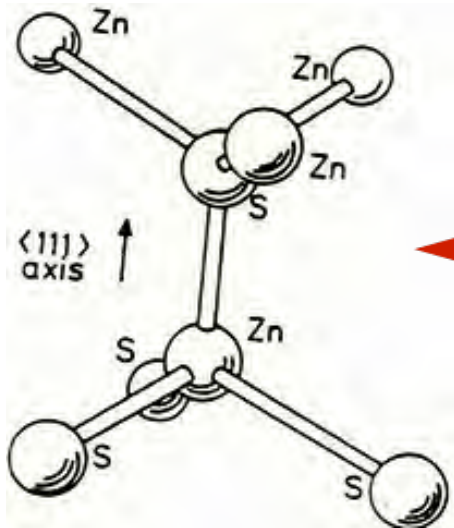


other views of the cubic unit cell

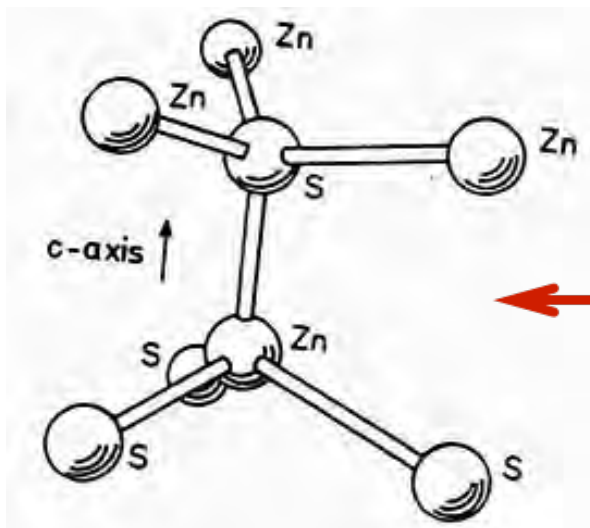


Diamond
Zincblende

- View of **tetrahedral coordination** & **2 atom basis**:



Zincblende \equiv face centered
cubic (**fcc**) lattice, **2 atom**
basis



Wurtzite \equiv hexagonal close
packed (**hcp**) lattice, **2 atom**
basis

- **Diamond & zincblende crystals:** Primitive lattice is **fcc**.

The **fcc** primitive lattice is generated by

$$\vec{r} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3.$$

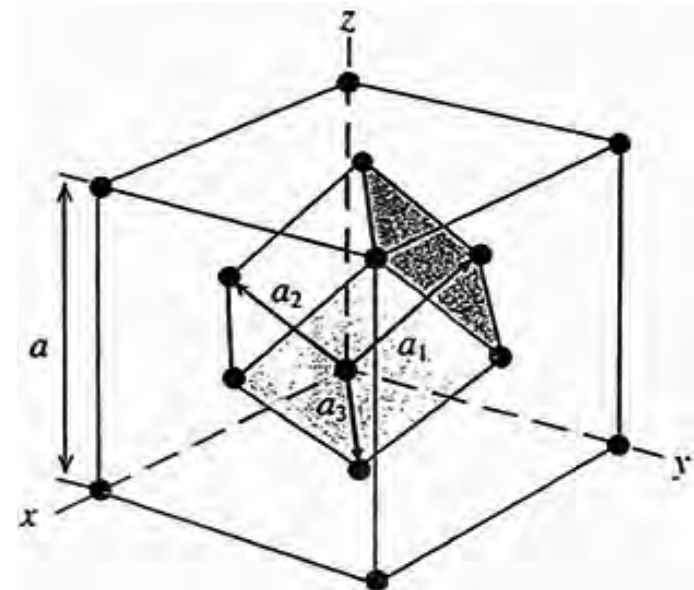
- The **fcc** primitive lattice vectors are:

$$\vec{a}_1 = (\frac{1}{2})a(0,1,0), \quad \vec{a}_2 = (\frac{1}{2})a(1,0,1), \quad \vec{a}_3 = (\frac{1}{2})a(1,1,0)$$

NOTE: The \vec{a}_i 's are NOT mutually orthogonal!

Primitive fcc lattice

cubic unit cell



Diamond:

2 identical atoms per fcc point

Zincblende:

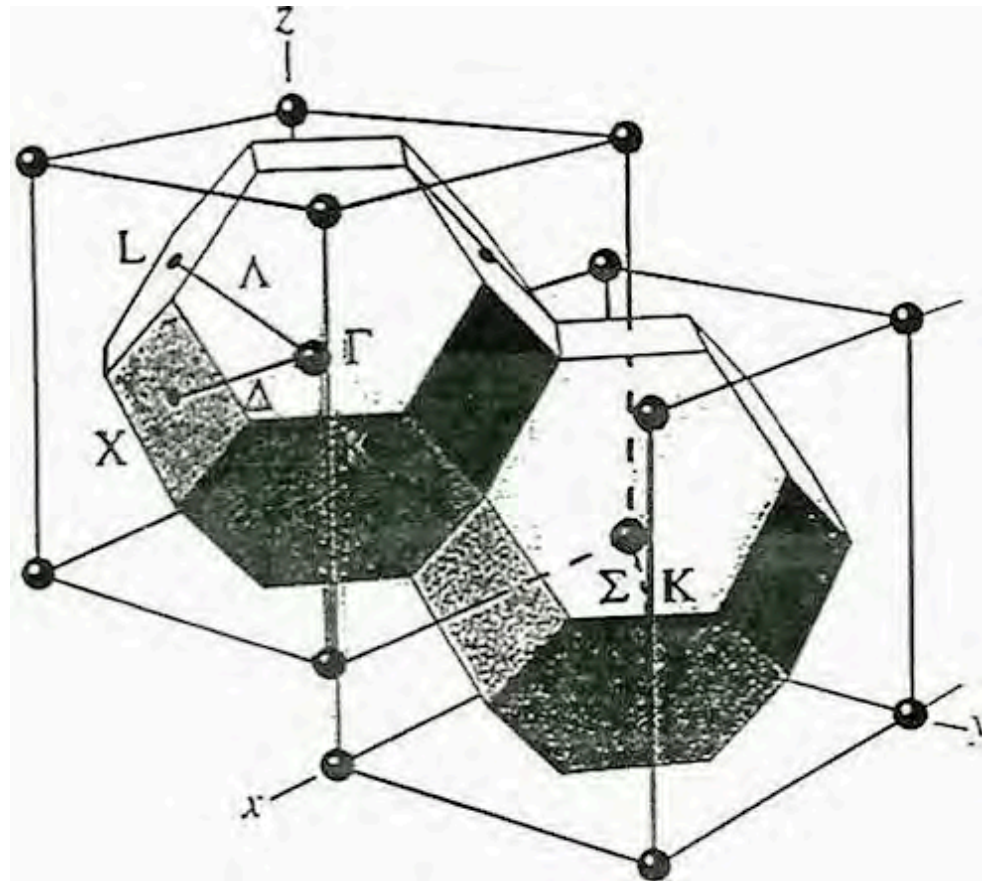
2 different atoms per fcc point

- **The 1st Brillion for the fcc lattice** (the primitive cell for the \vec{b} cc k space lattice) looks like:

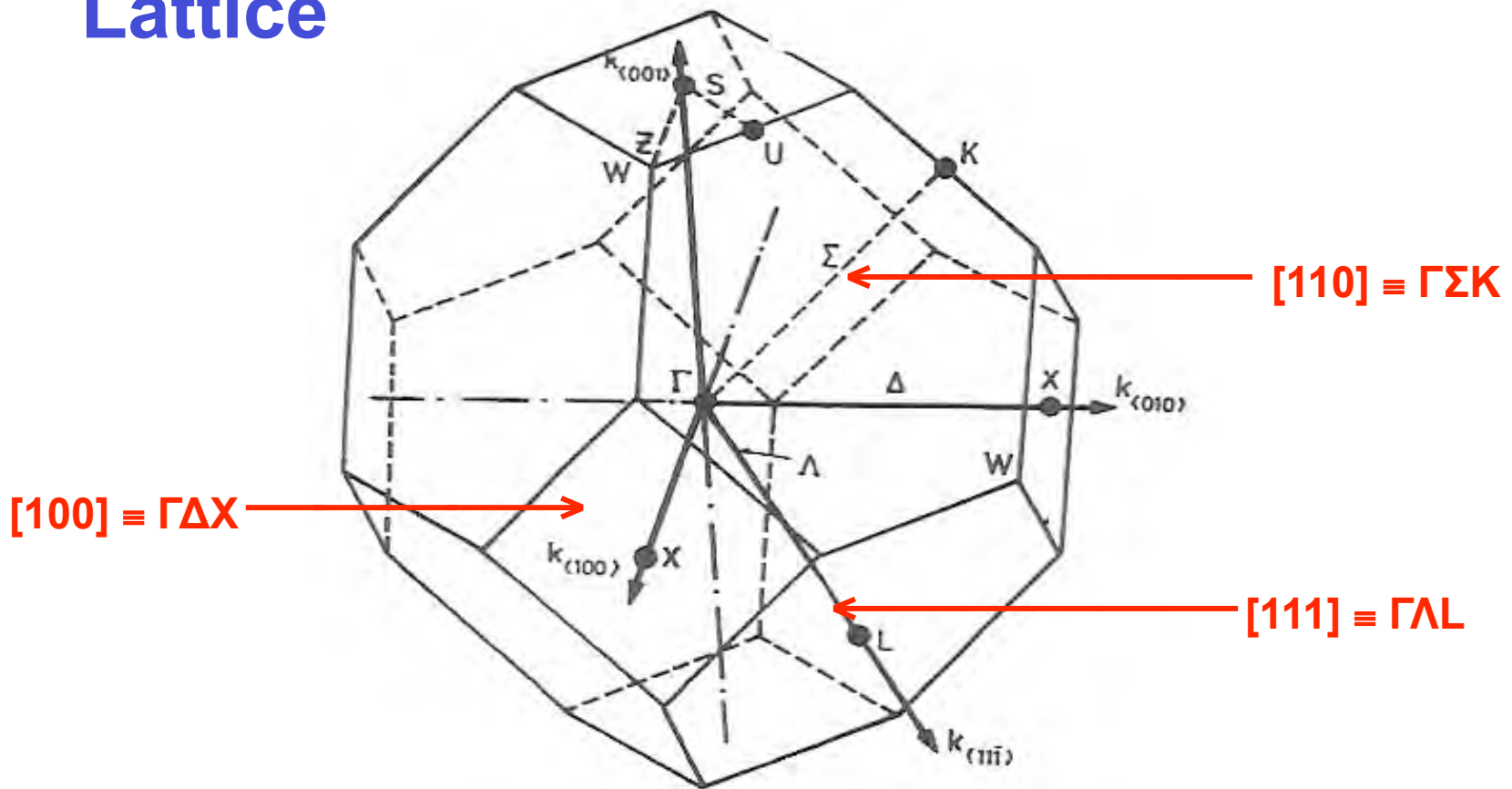
$$\vec{b}_1 = 2\pi(-1,1,1)/a$$

$$\vec{b}_2 = 2\pi(1,-1,1)/a$$

$$\vec{b}_3 = 2\pi(1,1,1)/a$$



Detailed View of BZ for Zincblende Lattice



To understand & interpret bandstructures, you need to be familiar with the high symmetry directions in this BZ!

PARTICLE/WAVE BASEBALL



Nada

Schrödinger's Wave Equation

1. Electron in Free Space

$$\left[\frac{\partial^2}{\partial x^2} + \frac{2m}{\hbar^2} (E - V(x)) \right] \psi(x) = 0$$

- Solve for particle moving in +x

$$\psi(x, t) = A \exp [i(kx - \omega t)]$$

with

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

$$\text{Note: } \lambda = \frac{h}{p} \quad \rightarrow \quad \lambda = \frac{h}{\sqrt{2mE}}$$

So, electron is a plane wave
with

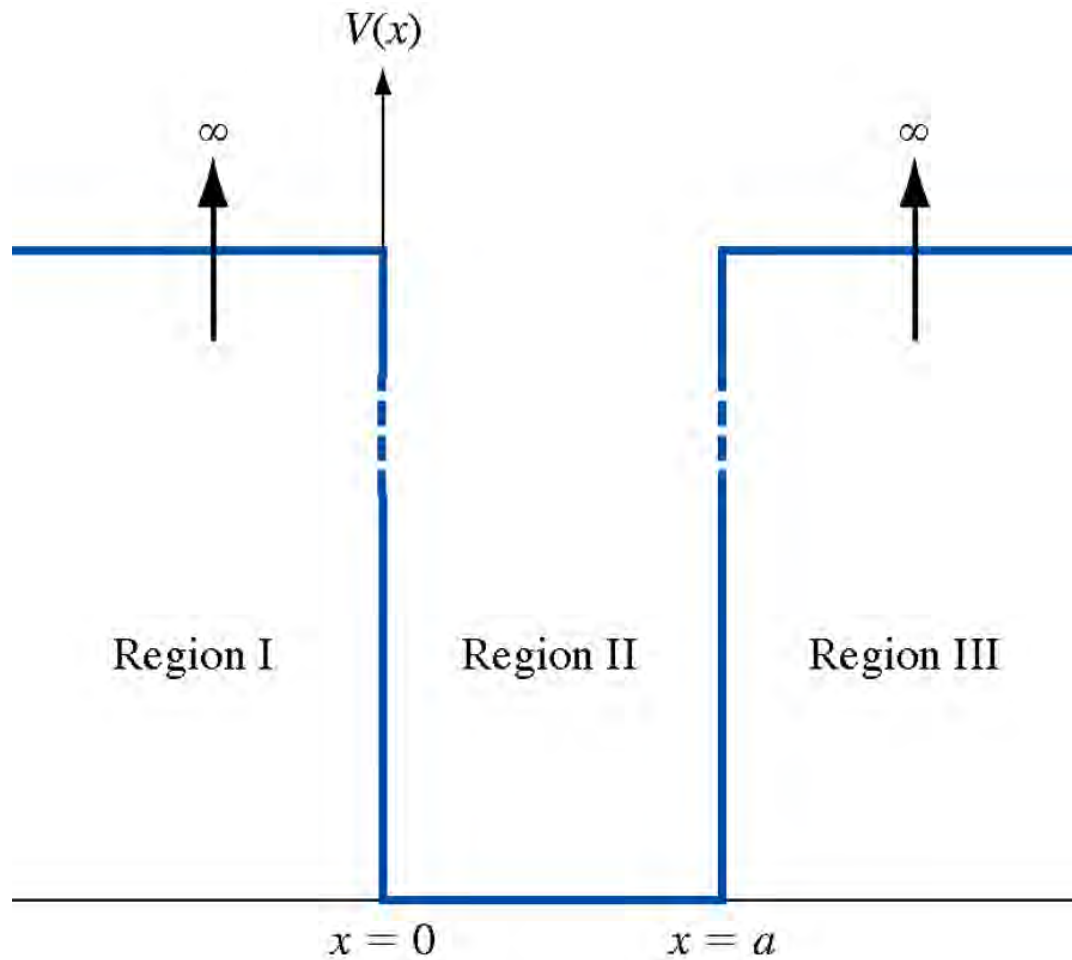
$$\psi(x, t)\psi^*(x, t) = AA^*$$

A constant!.... (exists everywhere in space)

But this means that momentum is well defined

And this leads to the notion of a wave packet

2. Infinite Well



Schrödinger's Wave Equation

$\psi = 0$ outside the well (regions I, III)

ψ and its derivative are continuous

$$\left[\frac{\partial^2}{\partial x^2} + \frac{2m}{\hbar^2} (E - V(x)) \right] \psi(x) = 0$$

For the infinite well, solution is

$$\psi(x) = A_1 \cos(kx) + A_2 \sin(kx)$$

$$\text{where } k = \sqrt{2m_0 E / \hbar^2}$$

Use boundary conditions @ $x = 0$, and a

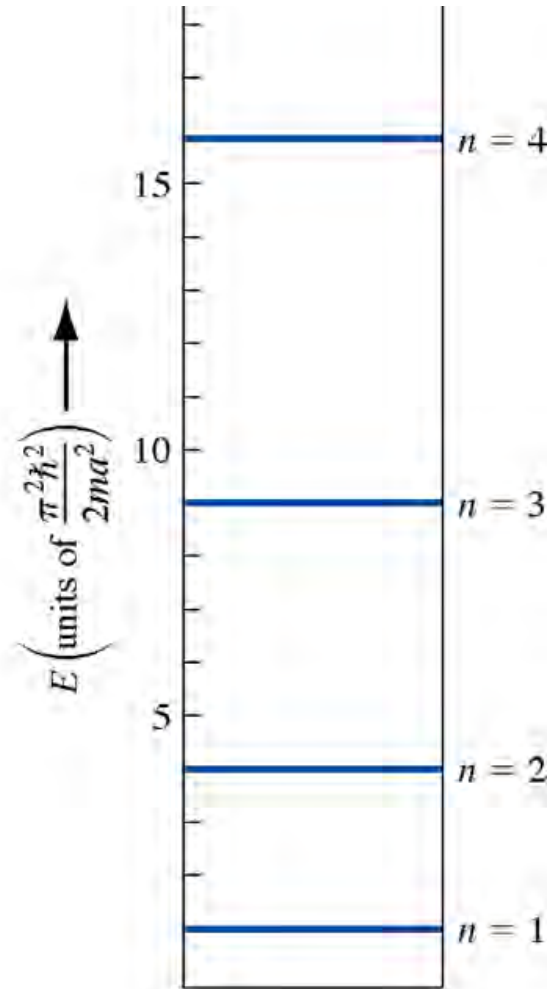
$$\text{at } x = 0, A_1 \cos(0) + A_2 \sin(0) = 0 \Rightarrow A_1 = 0$$

$$\text{at } x = a, A_2 \sin(ka) = 0 \Rightarrow ka = n\pi$$

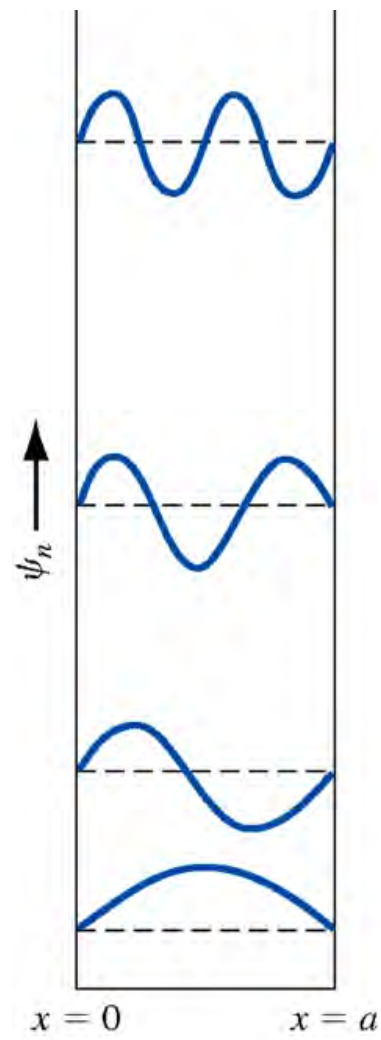
$$\text{hence } k = k_n = n \frac{\pi}{a} = \sqrt{2m_0 E_n / \hbar^2}; \text{ and}$$

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2m_0 a^2}$$

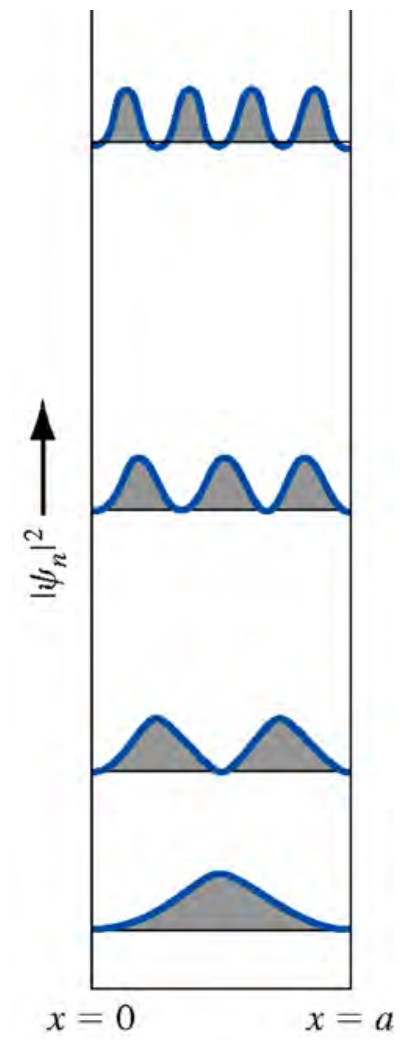
$$\psi(x) = \sqrt{\frac{2}{a}} \sin(k_n x)$$



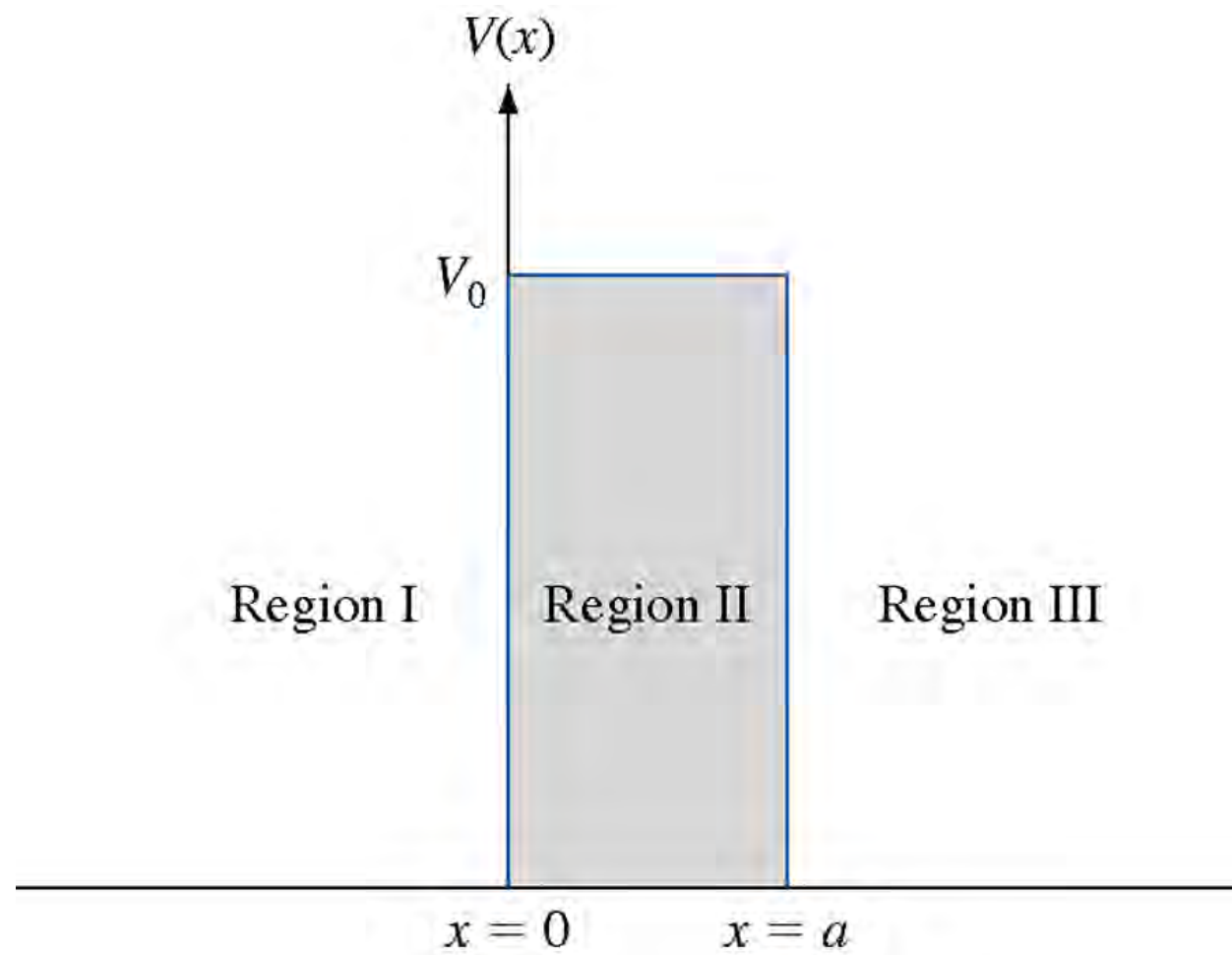
(a)



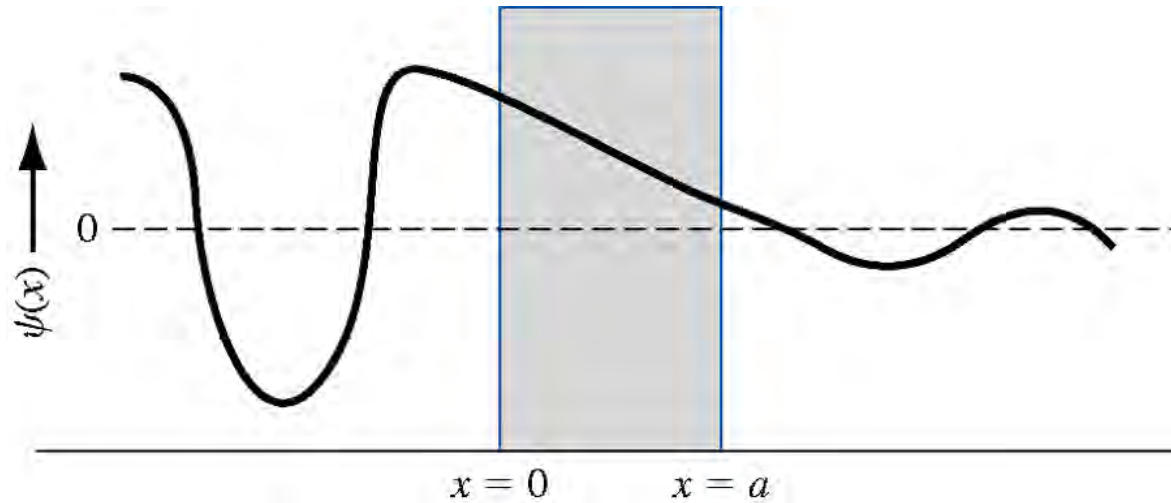
(b)



(c)



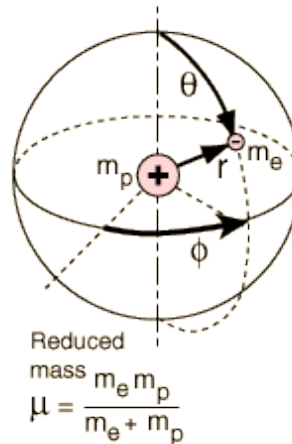
Electron Wave Function



$$\text{Transmission Coefficient } T \approx 16 \left(\frac{E}{V_0} \right) \left(1 - \frac{E}{V_0} \right) \exp(-2k_2 a)$$

- **Hydrogen Schrödinger Equation**

- The electron in the [hydrogen atom](#) sees a spherically symmetric potential, so it is logical to use [spherical polar coordinates](#) to develop the [Schrodinger equation](#).



- The potential energy is simply that of a [point charge](#):

$$U(r) = \frac{-e^2}{4\pi\epsilon_0 r}$$

- The expanded form of the Schrödinger equation is:

$$\frac{-\hbar^2}{2\mu} \frac{1}{r^2 \sin \theta} \left[\sin \theta \frac{\partial}{\partial r} \left(r^2 \frac{\partial \Psi}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Psi}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2 \Psi}{\partial \phi^2} \right] - U(r) \Psi(r, \theta, \phi) = E \Psi(r, \theta, \phi)$$

- Solving it involves [separating the variables](#) into the form

$$\Psi(r, \theta, \phi) = R(r)P(\theta)F(\phi)$$

$$\Psi(r, \theta, \phi) = R(r)P(\theta)F(\phi)$$

n

principal
quantum
number

ℓ

orbital
quantum
number

m_ℓ

magnetic
quantum
number

Electron Energy is derived as

$$E_n = - \frac{m_0 e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n^2}$$

The 3 quantum numbers are:

$$n = 1, 2, 3, \dots$$

$$l = n-1, n-2, n-3, \dots, 0$$

$$|m| = l, l-1, \dots, 0$$

Spin is the 4th quantum number.

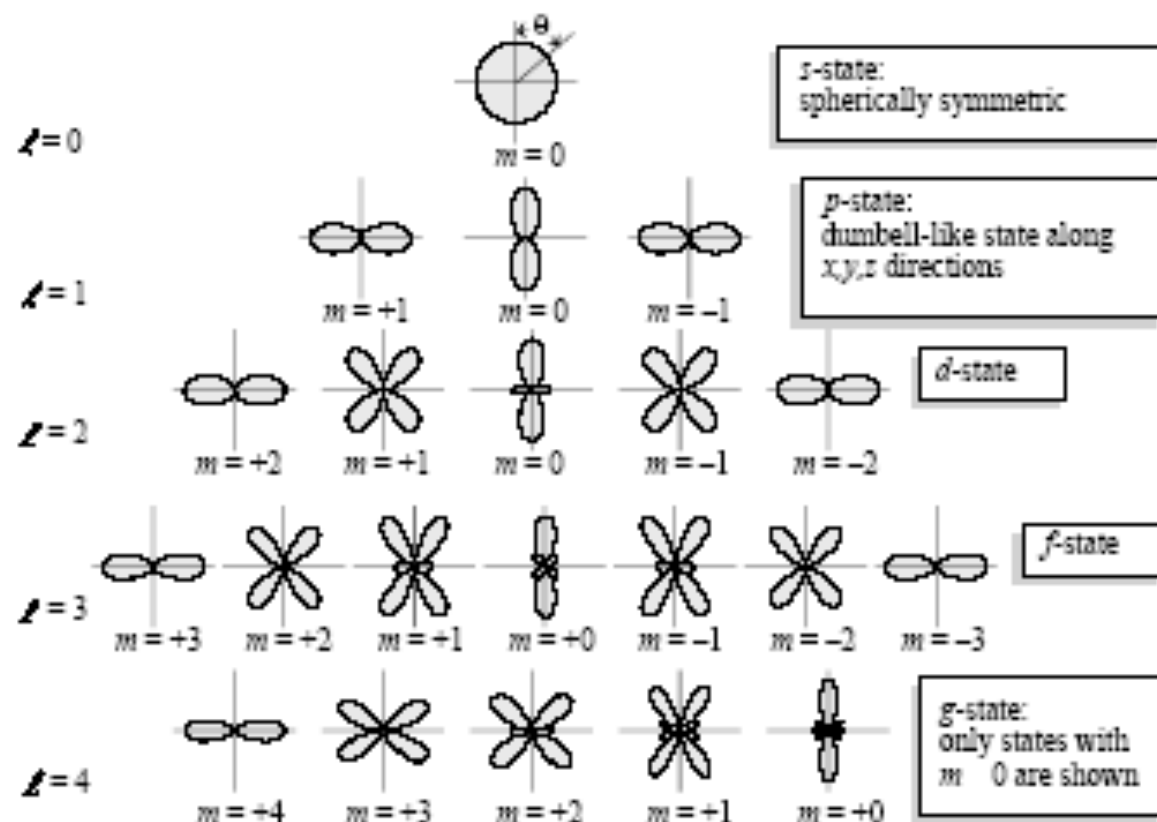
There is one electron state for each set
of 4 quantum numbers

NATURE OF ATOMIC FUNCTIONS:

These are important, since the cell periodic part of Bloch states is often made up of atomic-like states

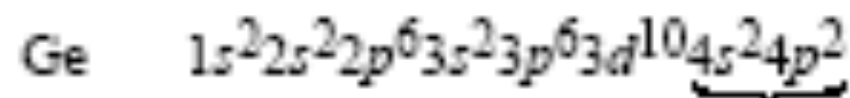
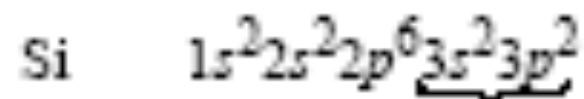
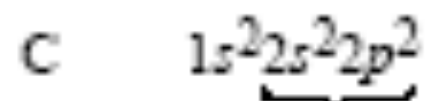
$l=0$: angular momentum is zero; called *s*-state

$l=1$: angular momentum is one (\hbar); called *p*-state

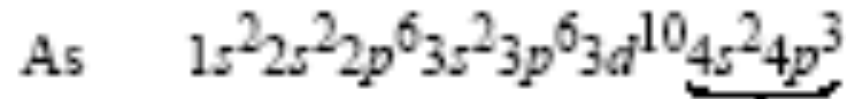
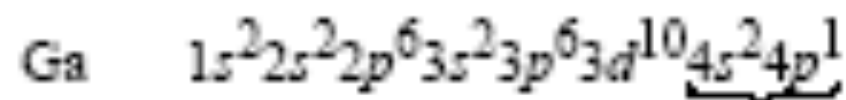


A plot of the probability density function of electronic states in an atom as a function of the angle θ for the *s, p, d, f, g* electrons.

IV Semiconductors

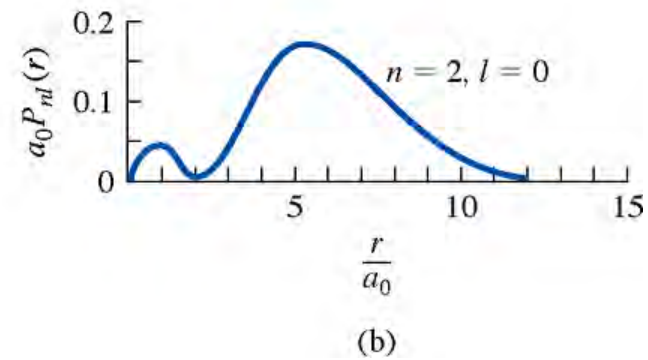
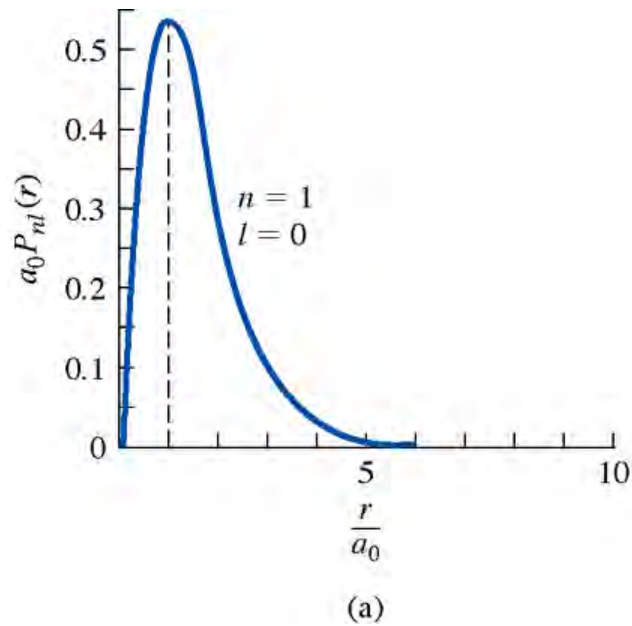


III-V Semiconductors



Outermost atomic levels are either *s*-type or *p*-type.

Radial Probability Density Function for a hydrogen atom



$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_0e^2} = 0.529 \text{ \AA}$$