

# Crystal Symmetry

# Crystal Structure

- Crystalline vs. amorphous
  - Diamond
  - graphite

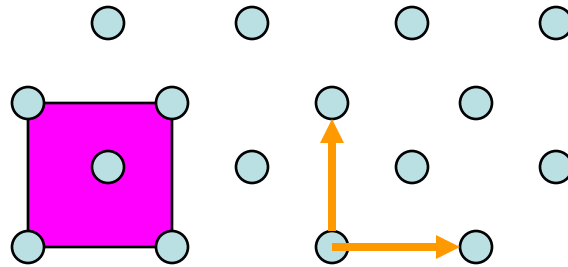


soot



- Binding
  - Covalent/metallic bonds (metals)
  - Ionic bonds (insulators)
- Crystal structure determines properties
  - Binding, atomic density, scattering
  - Symmetry controls properties of solids

# Periodic Structures



lattice: a periodic array of points in space.

-- The environment surrounding each lattice point is identical.

unit cell (volume): set of atoms that is repeated in lattice (not unique)

basis (vectors): Group of atoms “attached” to each lattice point in order to generate the crystal structure. (not unique)

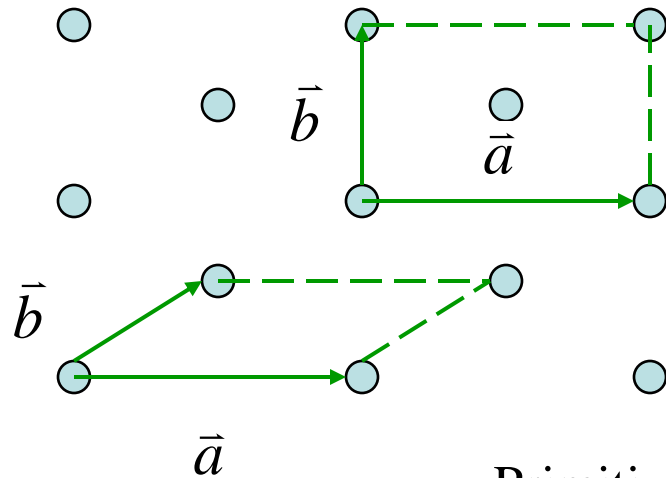
translational symmetry: base vectors or lattice vectors

Usually these vectors are chosen either:

- to be the shortest possible vectors, or
- to correspond to a high symmetry unit cell

# Example: 2-D cells

Movement of one translation vector = point of same symmetry (not unique)



Conventional (crystallographic) unit cell:  
larger than primitive cell; chosen to  
display high symmetry unit cell

Primitive unit cell: has minimum volume  
and contains only one lattice point

Unit cell defined by translation vectors

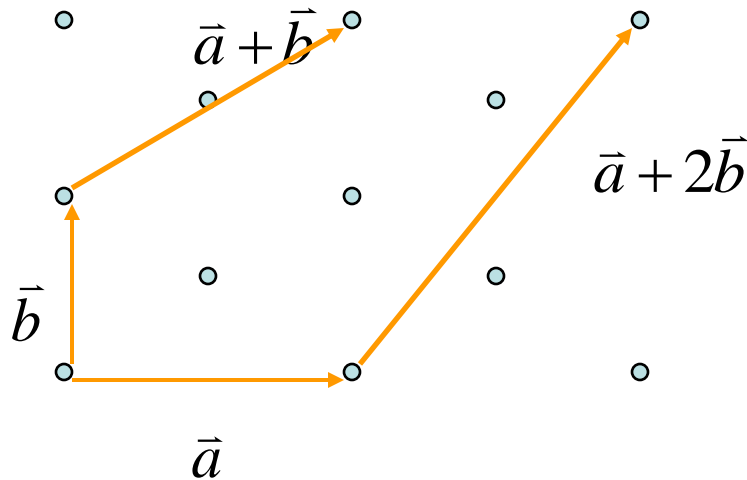
Many possible unit cells can explain symmetry

# Translation vectors and symmetry

A lattice translation vector connects two points in the lattice that have identical symmetry:

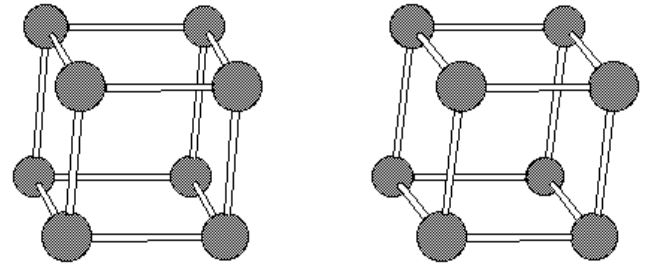
$$\vec{r} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c} \quad n_1 \ n_2 \ n_3 \in \text{integers}$$

In our 2-D lattice:

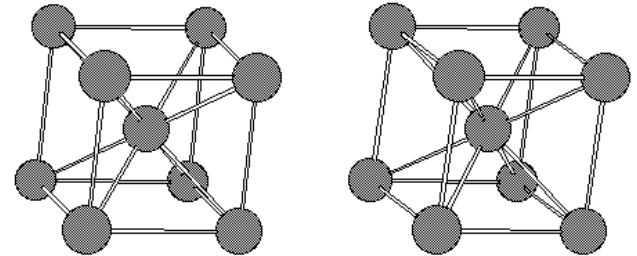


# Three dimensional cubic cells

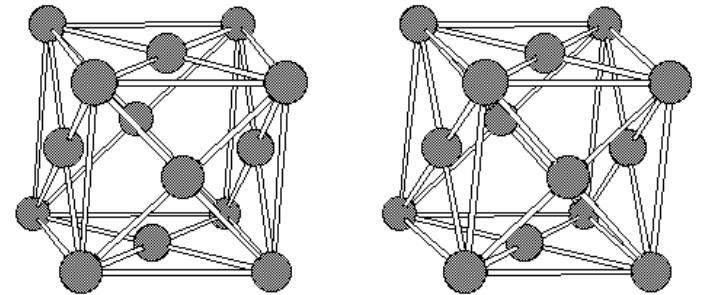
Simple Cubic structure



Body centered cubic structure



Face centered cubic structure

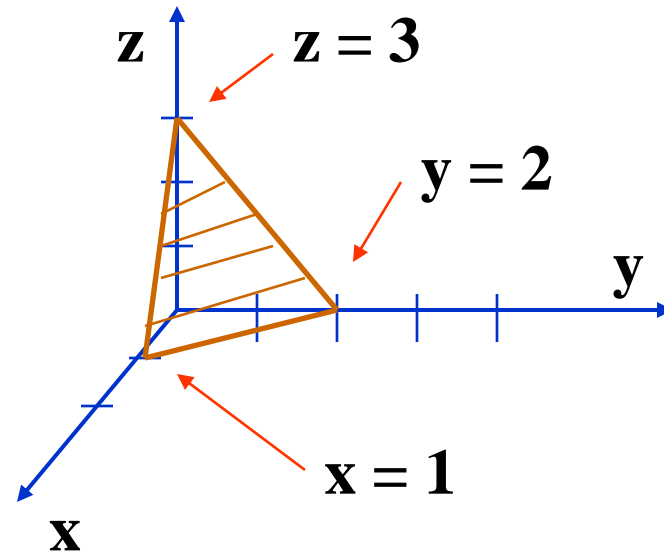


Hexagonal, etc....

# Miller Indices for Crystal Directions & Planes

Because crystals are usually anisotropic (their properties differ along different directions) it is useful to regard a crystalline solid as a collection of parallel planes of atoms. Crystallographers and CM physicists use a shorthand notation (Miller indices) to refer to such planes.

1. Determine intercepts ( $x$ ,  $y$ ,  $z$ ) of the plane with the coordinate axes



# Miller Indices Notation

**Express the intercepts as multiples of the base vectors of the lattice**

1. example, let's assume that the lattice is given by:  $\bar{a} = 1\hat{i}$     $\bar{b} = 1\hat{j}$     $\bar{c} = 3\hat{k}$

2. The intercept ratios become:  $\frac{x}{a} = \frac{1}{1} = 1$     $\frac{y}{b} = \frac{2}{1} = 2$     $\frac{z}{c} = \frac{3}{3} = 1$

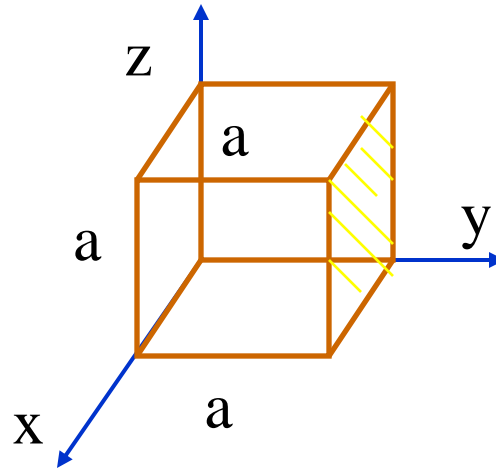
3. Form reciprocals:  $\frac{a}{x} = \frac{1}{1} = 1$     $\frac{b}{y} = \frac{1}{2}$     $\frac{c}{z} = \frac{1}{1} = 1$

4. Multiply through by the factor that allows you to express these indices as the lowest triplet of integers:

$2 \times (1 \frac{1}{2} 1) = (212)$    We call this the (212) plane.

# Another example

Find the Miller indices of the shaded plane in this simple cubic lattice:



$$\vec{a} = a\hat{i} \quad \vec{b} = a\hat{j} \quad \vec{c} = a\hat{k}$$

Intercepts:  $x = \infty$   $y = a$   $z = \infty$  non-intersecting  $\rightarrow$  intercept at  $\infty$

Intercept ratios:  $\frac{x}{a} = \infty$   $\frac{y}{a} = 1$   $\frac{z}{a} = \infty$

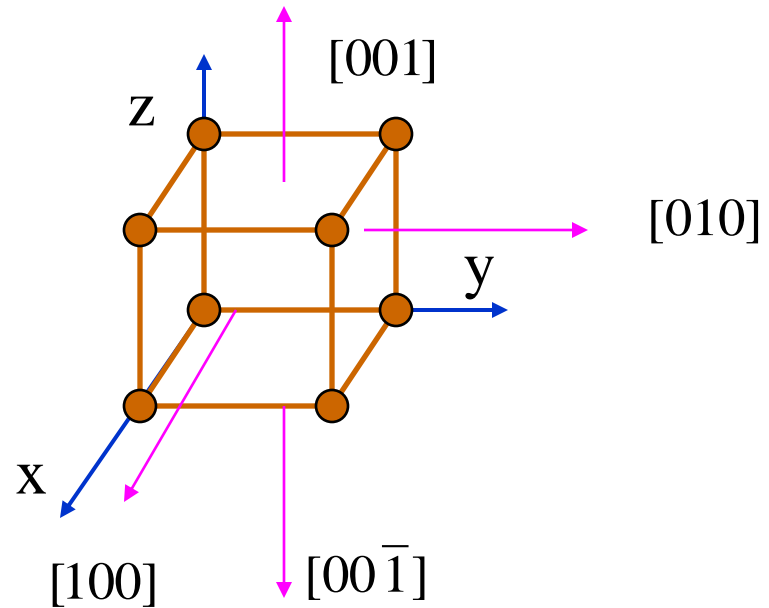
Reciprocals:  $\frac{a}{x} = 0$   $\frac{a}{y} = 1$   $\frac{a}{z} = 0$  We call this the (010) plane.

Note: (hkl) = a single plane; {hkl} = a family of symmetry-equivalent planes

# Crystal Planes and Directions

Crystal directions are specified  $[hkl]$  as the coordinates of the lattice point closest to the origin along the desired direction:

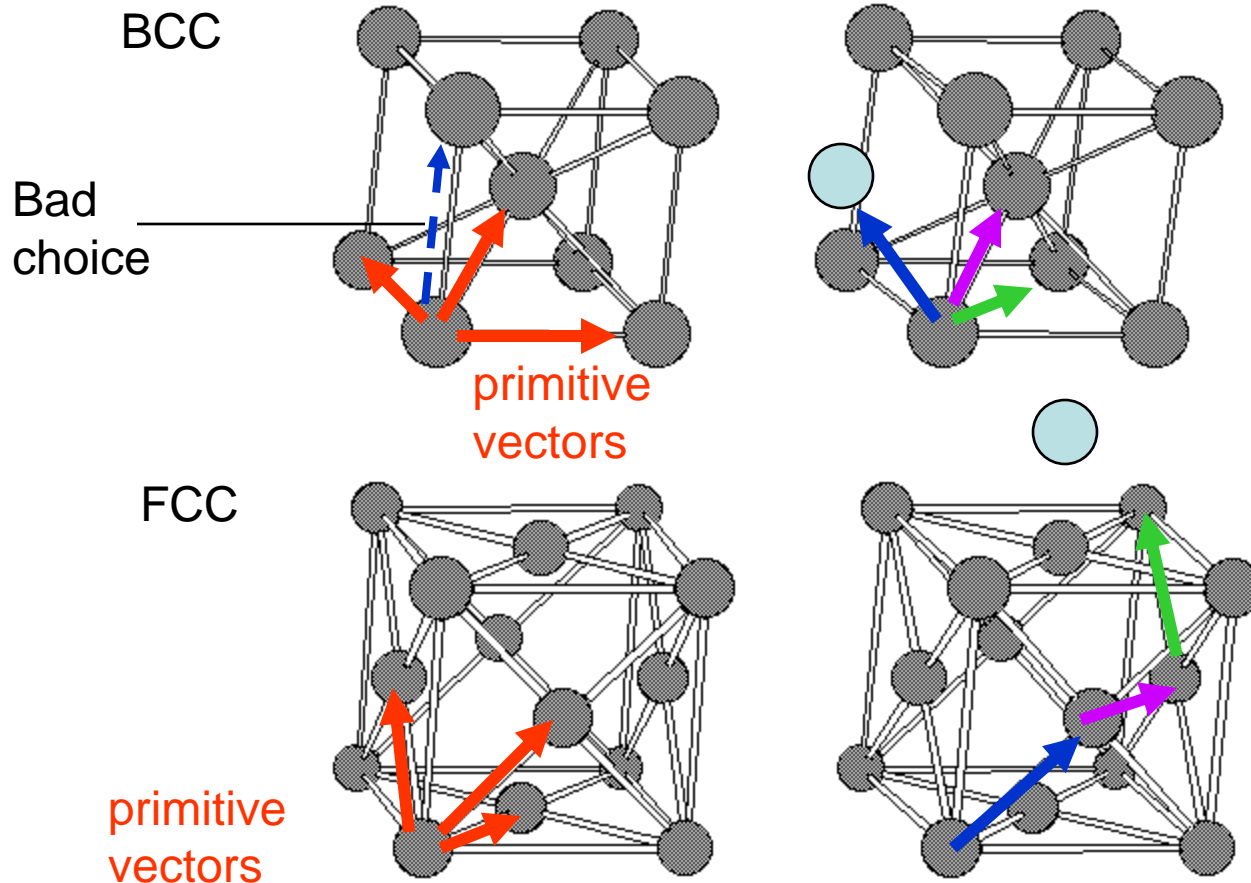
Note:  $[hkl]$  = a specific direction;  
 $\langle hkl \rangle$  = a family of symmetry-equivalent directions



Note that for cubic lattices, the direction  $[hkl]$  is perpendicular to the  $(hkl)$  plane

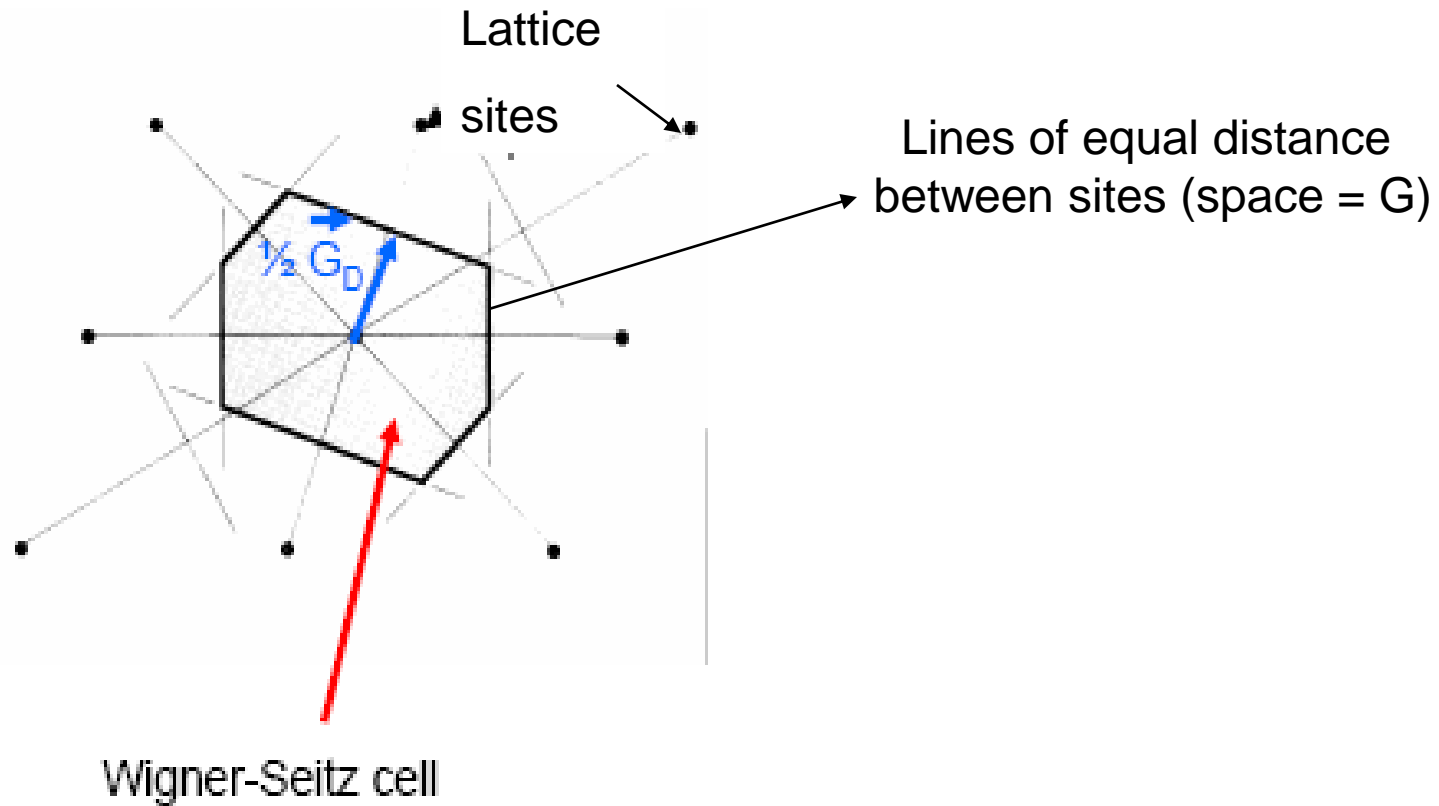
# Primitive Vectors

- Primitive vectors define translation symmetry of cube
- There are many other periodic vectors in 3-D crystal structure:
- Set of primitive vector translations will get to any atom



- Symmetry of electrons must match symmetry of crystal

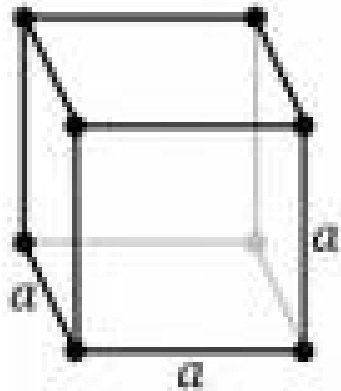
# Primitive Unit cell (2D): Wigner Seitz Cell



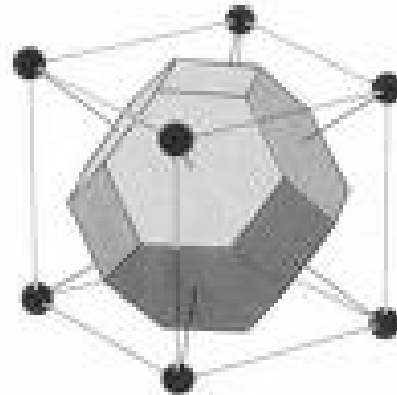
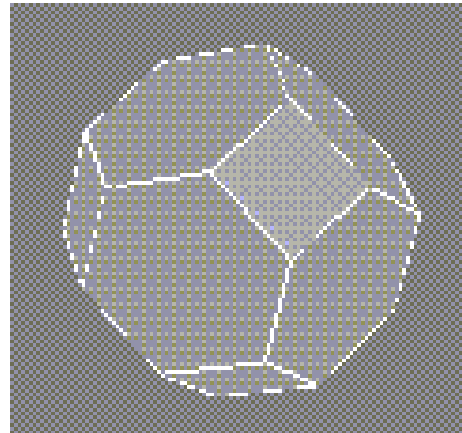
# Wigner Seitz Cells

Cubic  
Wigner Seitz Cell

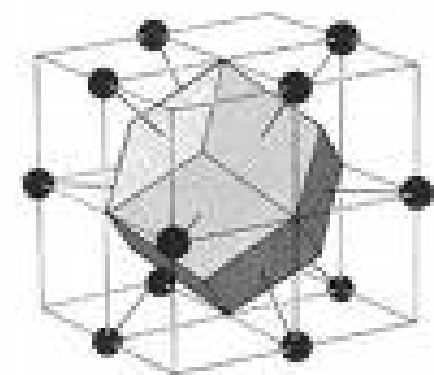
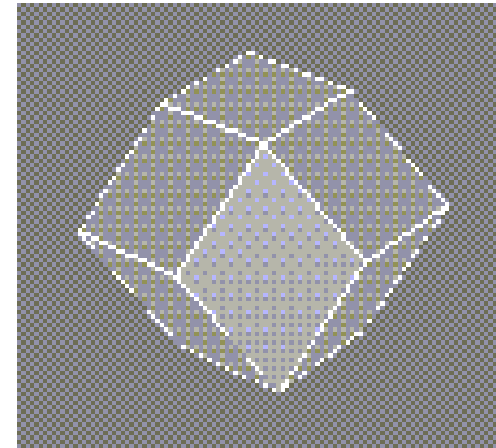
?



BCC  
Wigner Seitz Cell



FCC  
Wigner Seitz Cell



# Reciprocal Space

(x-ray scattering, electron waves)

- Lattice has periodicity in  $\mathbf{R}$  such that

$$e^{i\mathbf{K}\cdot(\mathbf{r}+\mathbf{R})} = e^{i\mathbf{K}\cdot\mathbf{r}} \quad \text{K and R are 3-D vectors}$$

- Reciprocal lattice will satisfy condition:

$$e^{i\mathbf{K}\cdot\mathbf{R}} = 1$$

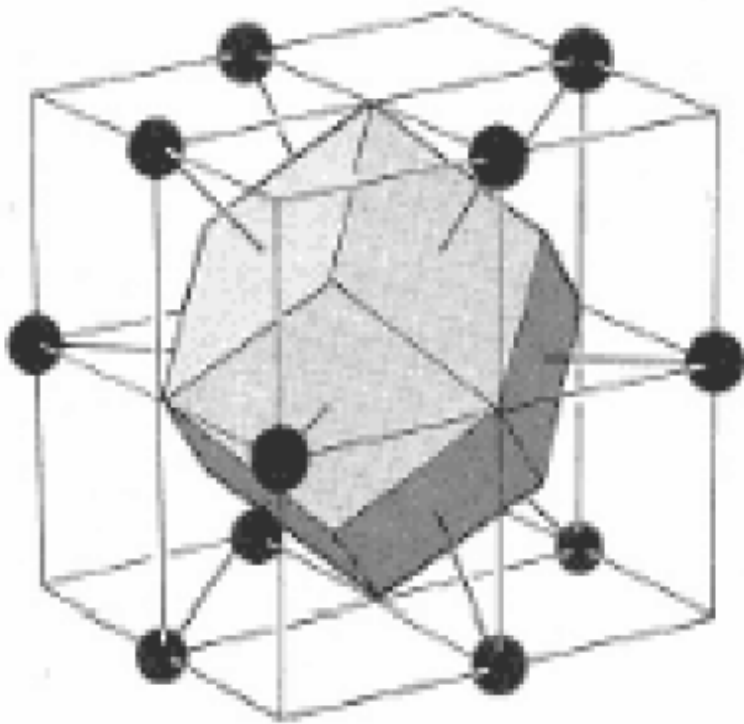
- Translate unit cell vectors to reciprocal space (k-space)

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \quad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \quad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

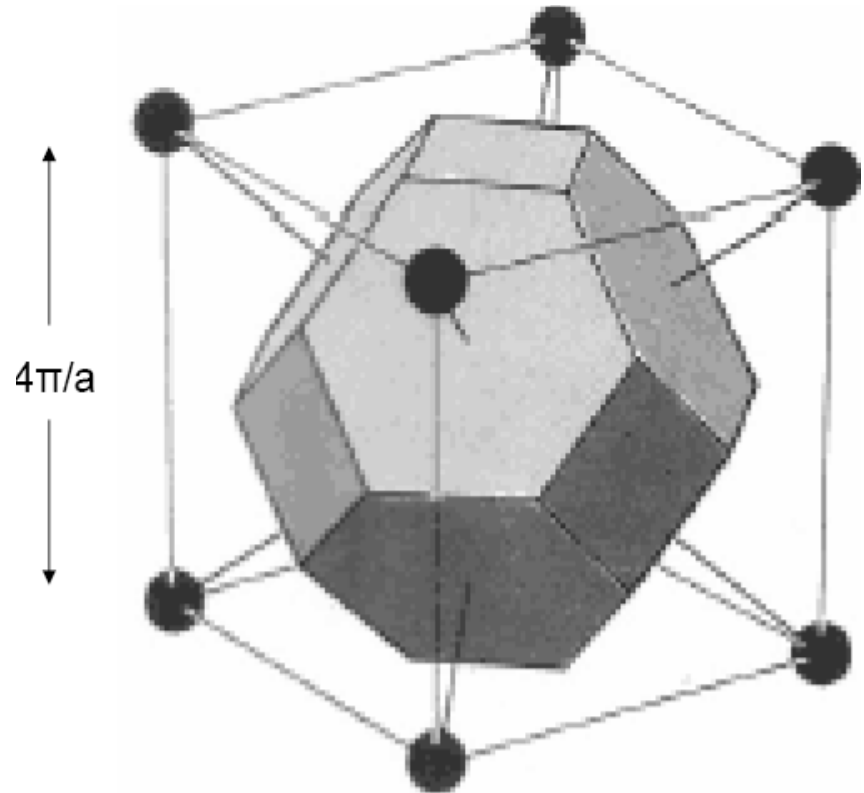
- Lattice of allowed k-vectors for Bloch waves

# Cubic lattice in Reciprocal space

BCC in real space  
FCC in reciprocal space



FCC in real space  
BCC in reciprocal space



# Bloch Waves

- Electron wave function (Schrodinger equation)

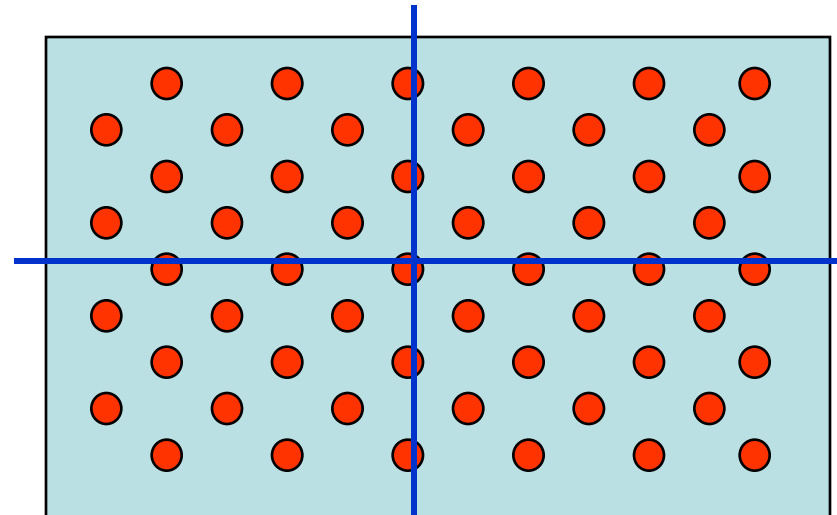
$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r) = \varepsilon \psi(r)$$

- Periodic Lattice boundary conditions

$$\psi(x, y, z) = \psi(x, y, z + L)$$

$$\psi(x, y, z) = \psi(x, y + L, z)$$

$$\psi(x, y, z) = \psi(x + L, y, z)$$

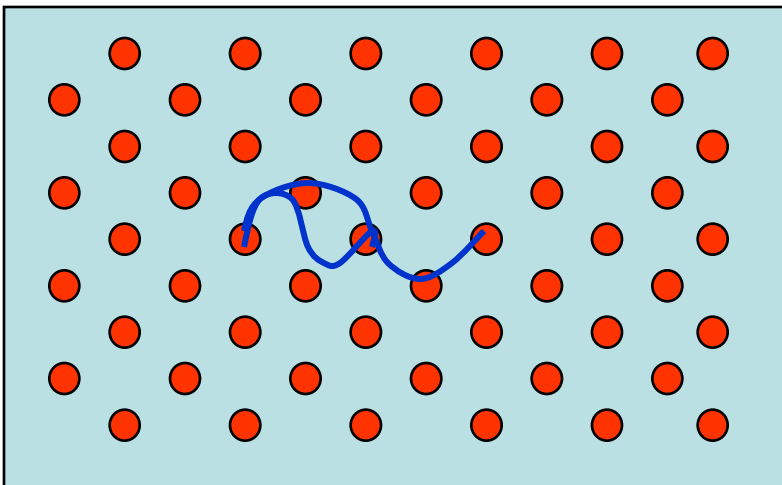


# Energy levels

- Solution in periodic lattice

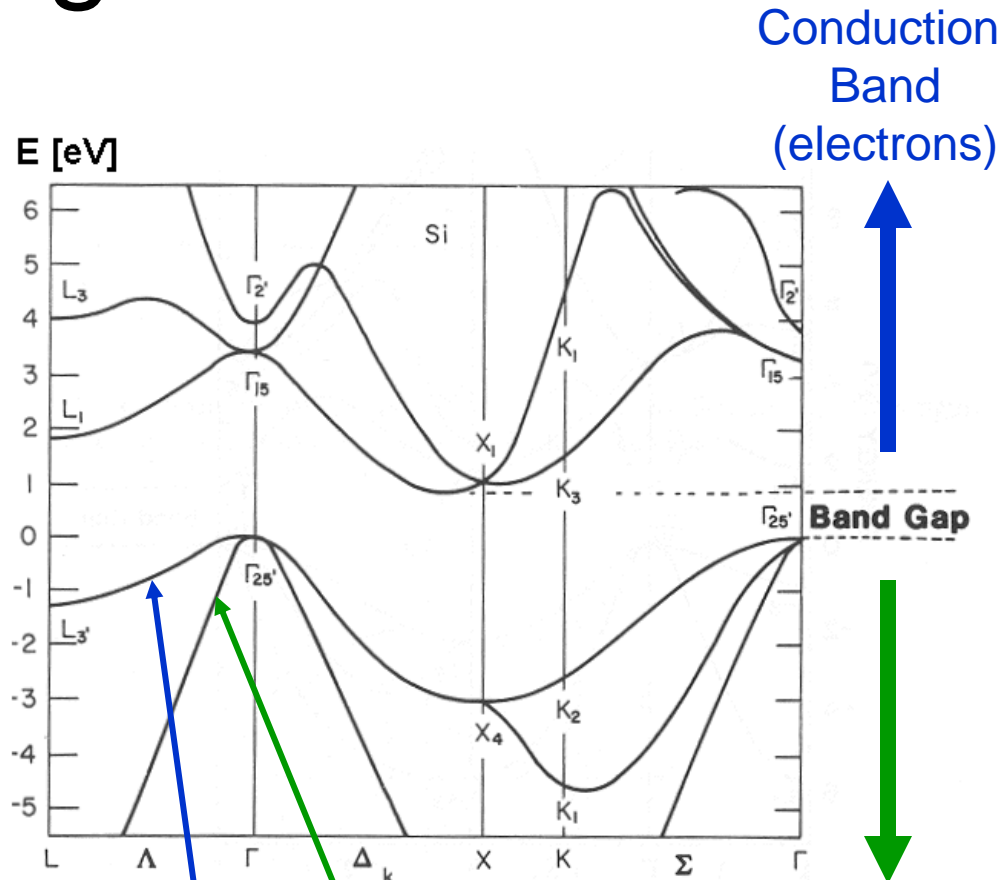
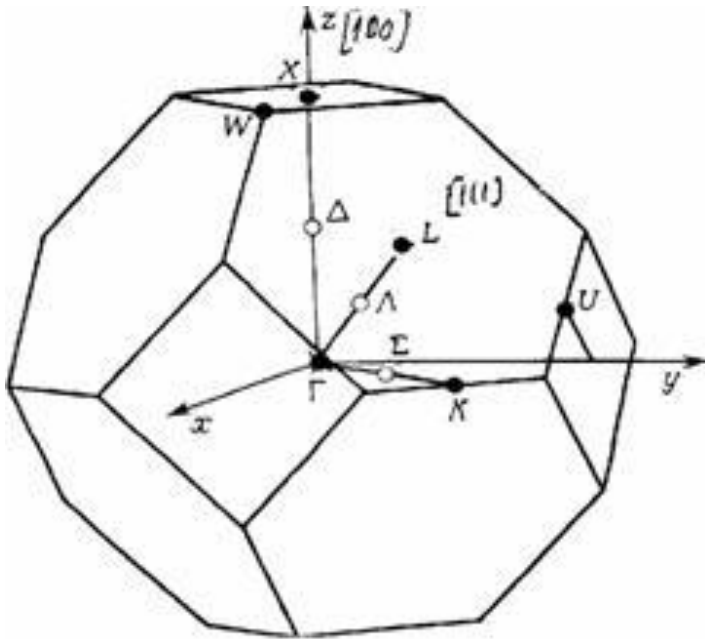
$$\psi_k(r) = \frac{1}{\sqrt{V}} e^{ik \cdot r}$$

$$k_x = \frac{2\pi n_x}{L}, k_y = \frac{2\pi n_y}{L}, k_z = \frac{2\pi n_z}{L}$$



$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m}$$

# Band Diagram of Si



Conduction Band (electrons)

Band Gap

Valence Band (holes)

Effective Mass ~ slope

$$\frac{1}{m^*} = \frac{1}{\hbar} \frac{\partial^2 \epsilon(k)}{\partial k_x \partial k_y}$$

Light holes

Heavy holes

# Can't make it smaller: push it

Effective mass  $\sim \frac{1}{m^*} = \frac{1}{\hbar} \frac{\partial^2 \varepsilon(k)}{\partial k_x \partial k_y} \sim a^2$  (lattice constant)

## Compressive Stress

**NMOS: Tensile SiN cap layer  
larger Si-Si**

**PMOS: Compressive SiGe layer  
smaller Si-Si  
(Ge = 11% larger than Si)**

## Increased mobility

**Change Si lattice constant**

Intel 65nm PMOS transistor

