CRYSTALLINE SOLIDS IN 3D

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PHY 491, October 7th, 2011

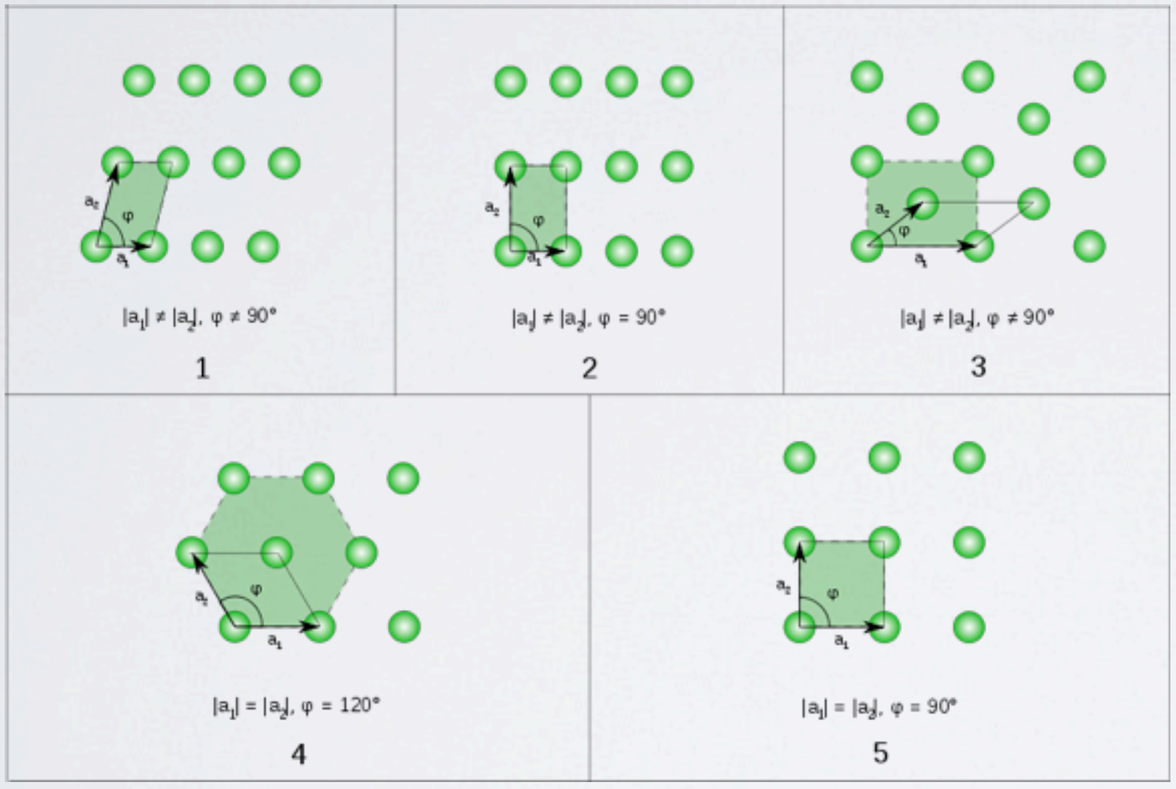
OVERVIEW

- First - are there any questions from the previous lecture?

- Today, we will answer the following questions:
  - *Why should we care about crystal structure?*
  - *How many Bravais lattices are there in 3D?*
  - *How do we describe them mathematically?*
  - *What are some common examples of these structures?*
  - *What are some not-so common examples?*

REVIEW OF 2D BRAVAIS LATTICES

- In ***2D***, we saw that there are ***5 distinct Bravais lattices***.
- Characterized by ***2 lattice vectors*** (2 magnitudes + 1 angle between vectors)



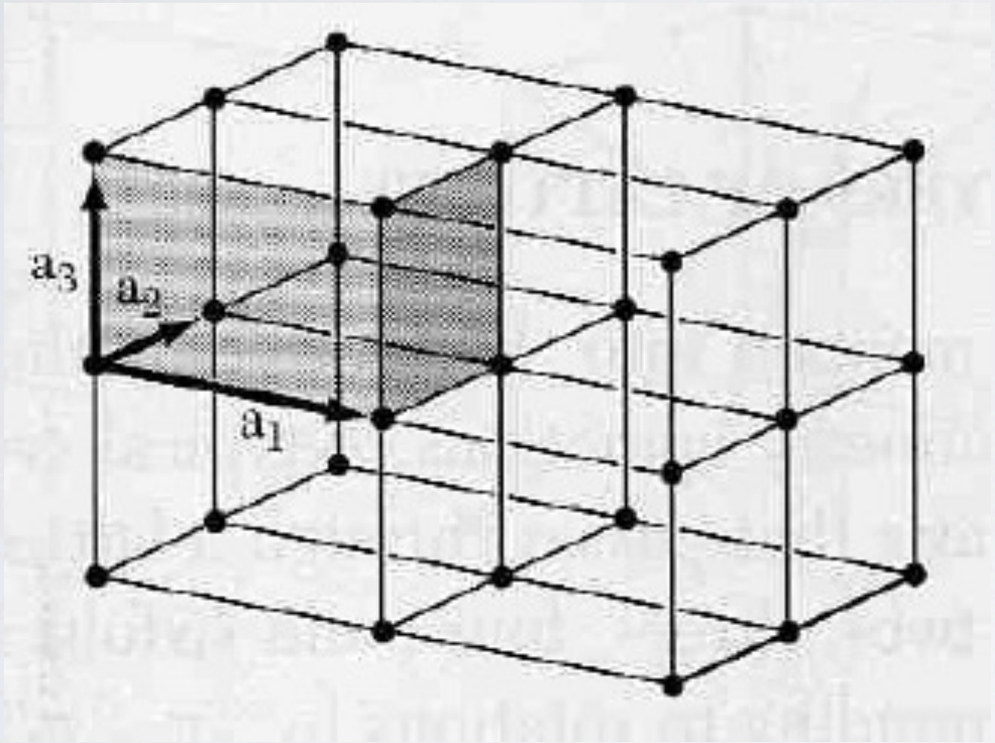
- 1 = oblique
- 2 = rectangular
- 3 = centered rectangular
- 4 = triangular net/hexagonal
- 5 = square net

- Recall that must assign a ***basis*** to the lattice to describe a real solid.

Image source: Wikipedia

3D BRAVAIS LATTICES

- In 3D, lattices are characterized by ***3 lattice vectors*** (3 magnitudes, 3 angles)



- There are 2 common conventions for labeling lattice vectors:
  - Kittel (your book) uses:
    - Vectors: ($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$)
    - Angles: ($\boldsymbol{\alpha}_{12}$, $\boldsymbol{\alpha}_{23}$, $\boldsymbol{\alpha}_{31}$)
    - $\boldsymbol{\alpha}_{12}$ is the angle b/w $\mathbf{a}_1$ and $\mathbf{a}_2$
  - Perhaps more common:
    - Vectors: ($\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$)
    - Angles: ($\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$)
    - $\boldsymbol{\alpha}$ is the angle b/w $\mathbf{b}$ and $\mathbf{c}$

- We find that there are ***14 distinct Bravais lattices***.
- These 14 can be divided further into ***7 lattice classes***

Image source: Kittel

3D BRAVAIS LATTICES (CONT.)

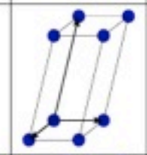
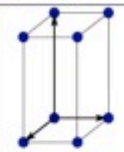
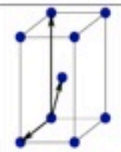
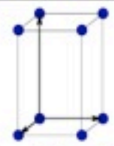
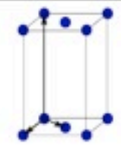
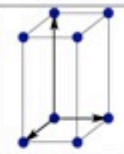
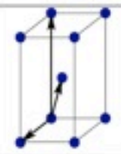
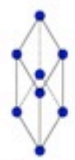
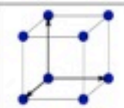
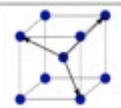
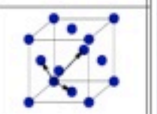
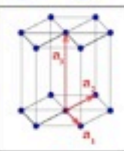
Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120°$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120°$ $\alpha_{23} = \alpha_{31} = 90°$				

Table 1.1: Bravais lattices in three-dimensions.

- ***7 lattice classes, 14 distinct Bravais lattices***
- You will also see 'volume centered' structures referred to as 'body centered'

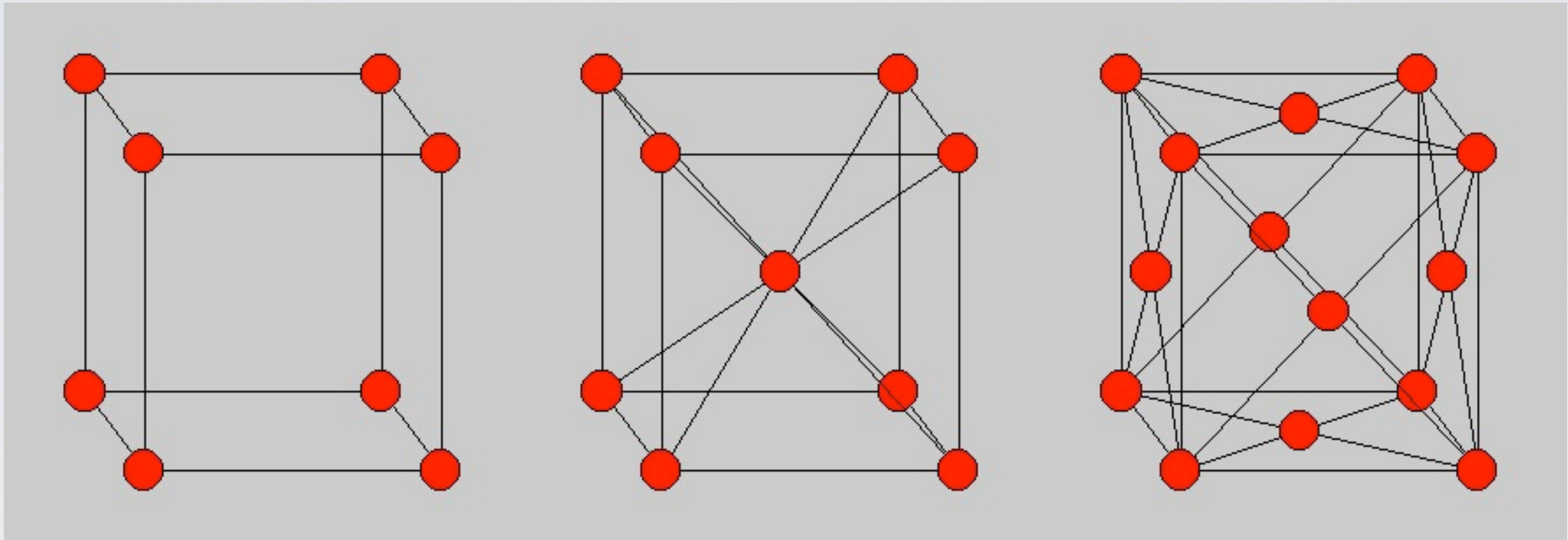
- There is an error in this table: trigonal refers to a crystal system, NOT a Bravais lattice. The Bravais lattice is actually called rhombohedral.

- For now, you will be most interested in the cubic lattice classes

- If you continue in condensed matter physics, you will probably encounter some of the more 'exotic' structures in your research

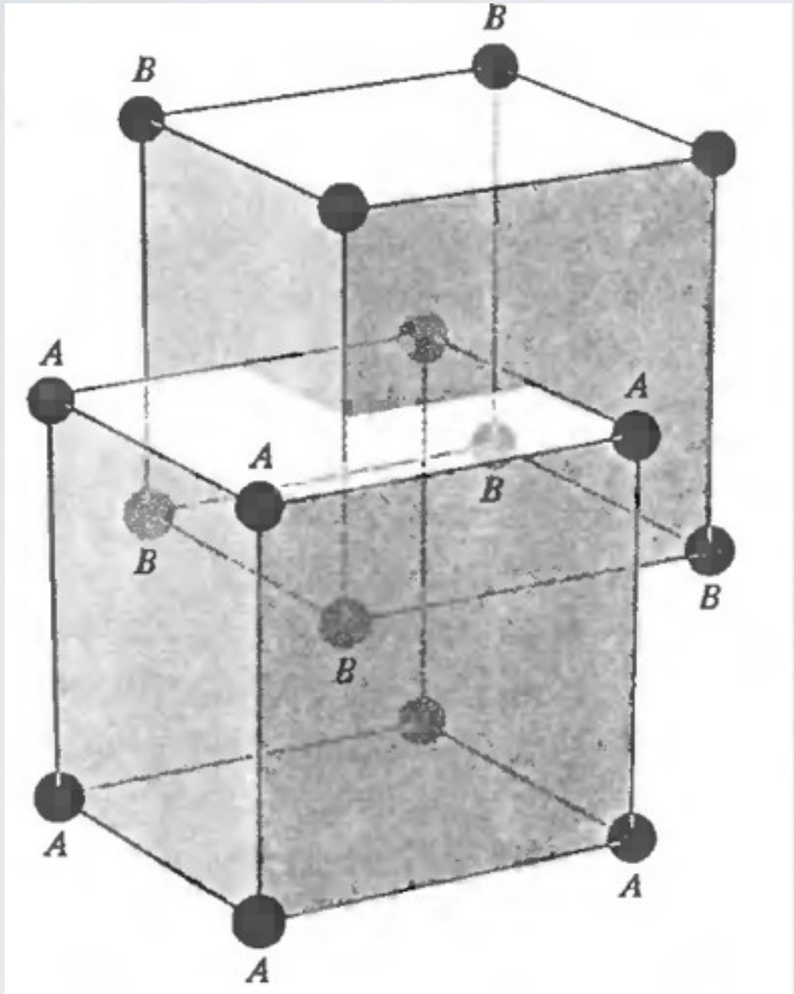
CUBIC BRAVAIS LATTICES

Left to right: ***simple***, ***body/volume centered***, ***face centered***



- You will often see the abbreviations ***sc***, ***bcc***, and ***fcc*** for these lattices.
- Assigning lattice vectors is, as in 2D, non-unique, but not all choices are equally useful.
- Let's consider a ***bcc*** example.

BODY CENTERED CUBIC EXAMPLE



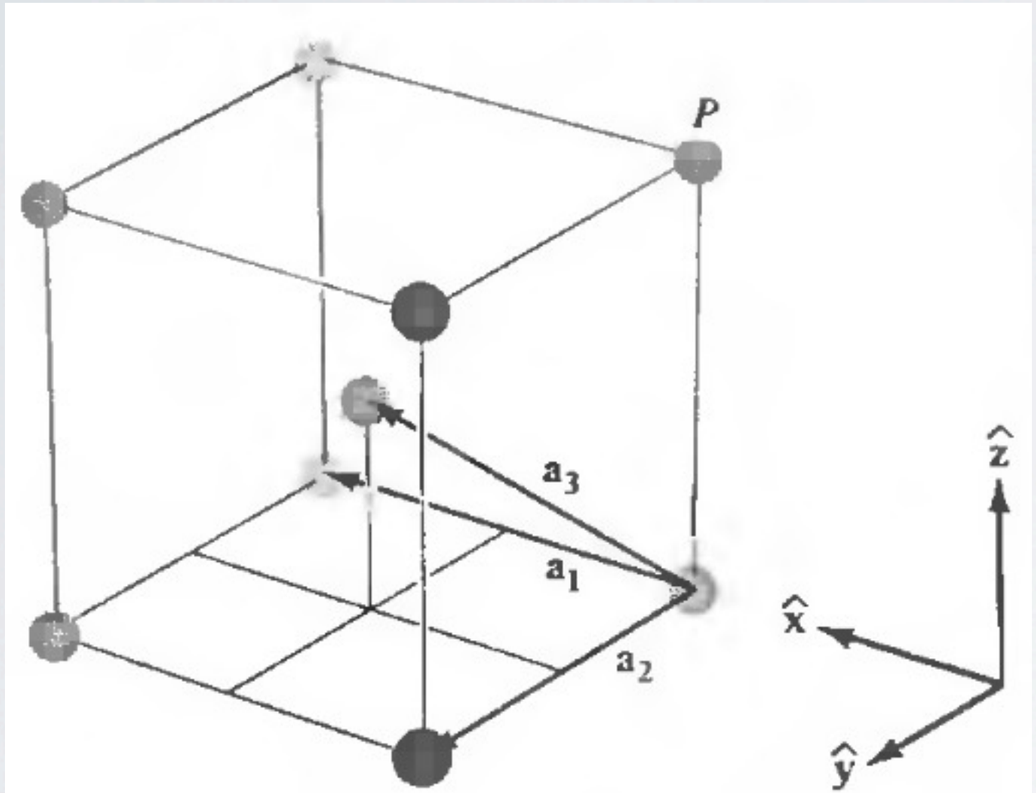
- We can conceptualize the bcc structure as ***2 interpenetrating sc structures***

- Vertices of a cube in one lattice lie at the center of the other

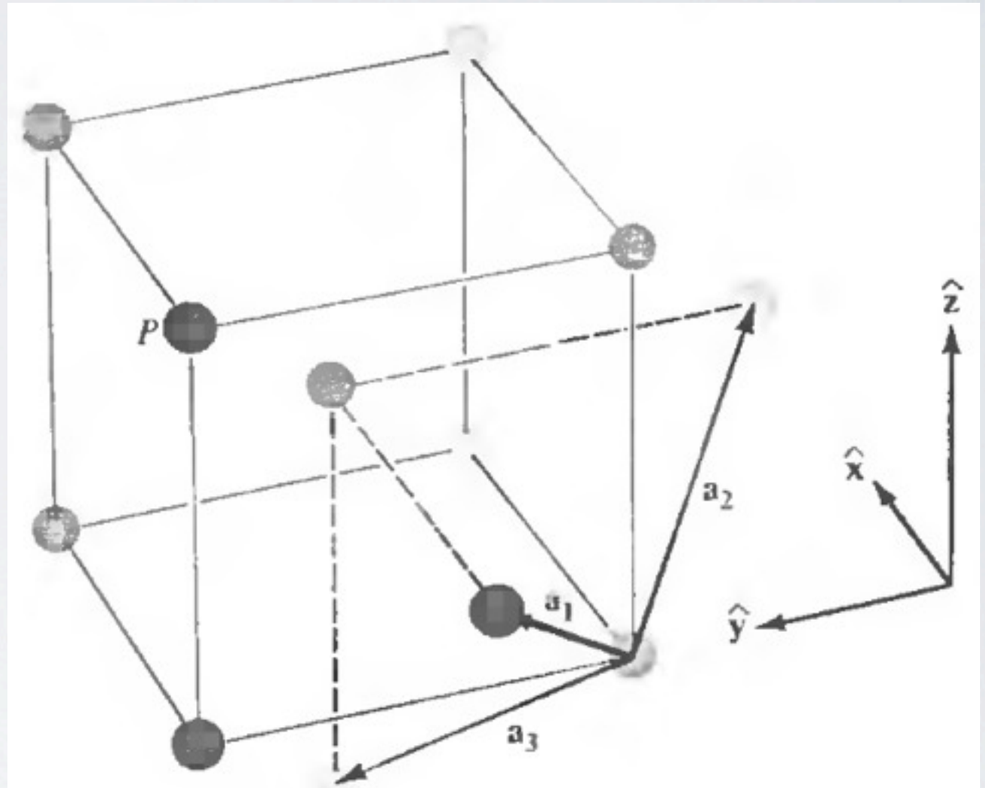
- Consider 2 choices of lattice vectors:
  - Origin at an ***A*** atom:
    - 2 vectors to other ***A*** atoms, 1 to a ***B*** atom
    - All 3 vectors to ***B*** atoms

- Let's codify this mathematically

BODY CENTERED CUBIC EXAMPLE (CONT).



$$\mathbf{a}_1 = a\mathbf{x}$$
$$\mathbf{a}_2 = a\mathbf{y}$$
$$\mathbf{a}_3 = a/2\ (\mathbf{x}+\mathbf{y}+\mathbf{z})$$



$$\mathbf{a}_1 = a/2\ (\mathbf{y}+\mathbf{z}-\mathbf{x})$$
$$\mathbf{a}_2 = a/2\ (\mathbf{z}+\mathbf{x}-\mathbf{y})$$
$$\mathbf{a}_3 = a/2\ (\mathbf{x}+\mathbf{y}-\mathbf{z})$$

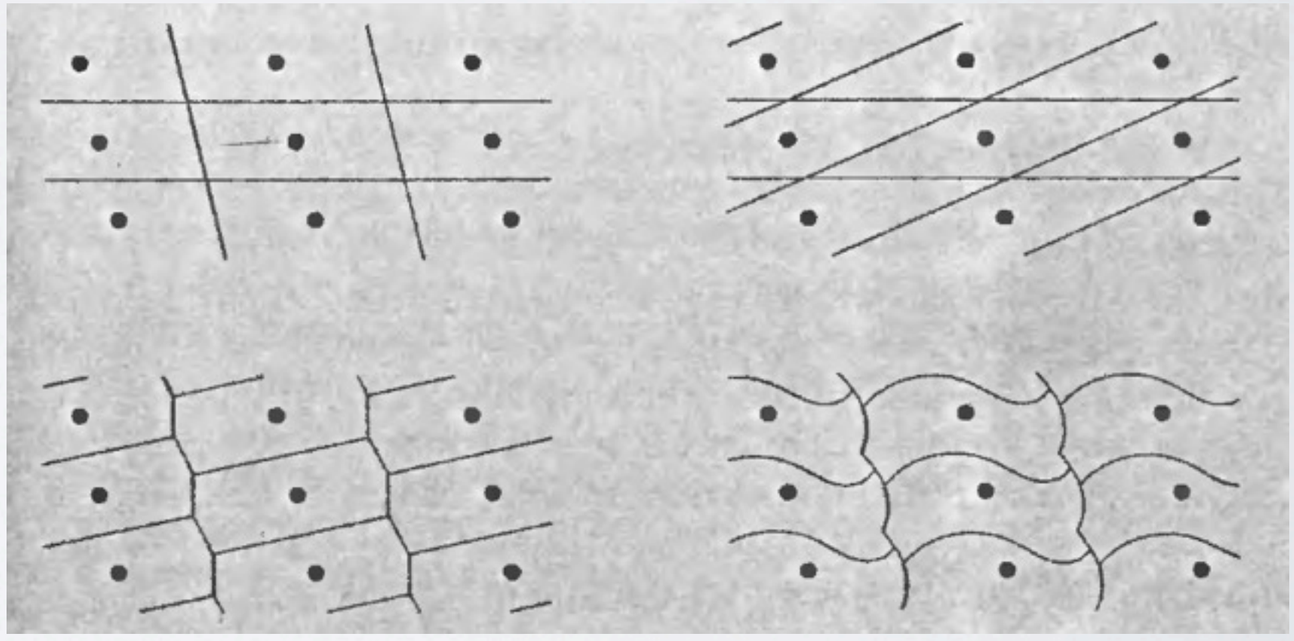
PRIMITIVE CELLS

- The ***unit cell*** is a volume that can fill all of space, without gaps, when translated by lattice vectors
- The choice of unit cell is also non-unique, so it is convenient to have a standard for assigning them.
- This is called the ***Wigner-Seitz cell,*** it is an example of a ***primitive cell***

- A ***primitive cell*** is the minimum volume of space the can be used to characterize a Bravais lattice that contains ***exactly 1 lattice point***.

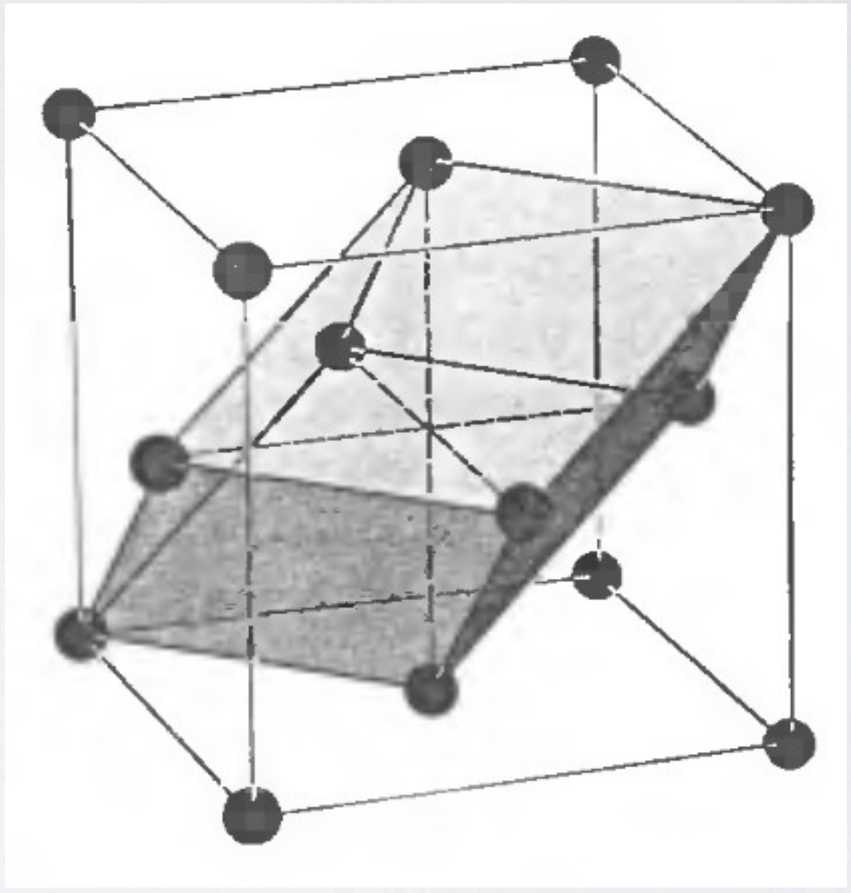
- This is, of course, also non-unique:

- Notice that many of the choices have symmetries that differ from the underlying lattice...



PRIMITIVE CELLS (CONT.)

- Things can look even weirder in 3D...
- The unshaded area is the ***conventional*** fcc unit cell.
- The shaded area is one choice of the primitive cell
- This may seem counter-intuitive: parallelepiped has 8 vertices, each of which 'contains' 1/8 of a lattice point - ***8 x 1/8 = 1 point per cell***
- Parallelepiped ***does NOT*** have the cubic symmetry of the original Bravais lattice...



WIGNER-SEITZ CELL

- We want a convenient standard for constructing ***primitive cells that preserve the symmetry of the original Bravais lattice***.
- Along came these 2 gentlemen...

- Eugene Wigner
- Hungarian theoretical physicist
- Nobel laureate (1963)
- Fun fact: Paul Dirac's brother-in-law

- Frederick Seitz
- Wigner's student
- Started big lab at UIUC
- Fun facts:
  - Global warming skeptic (before it was cool)

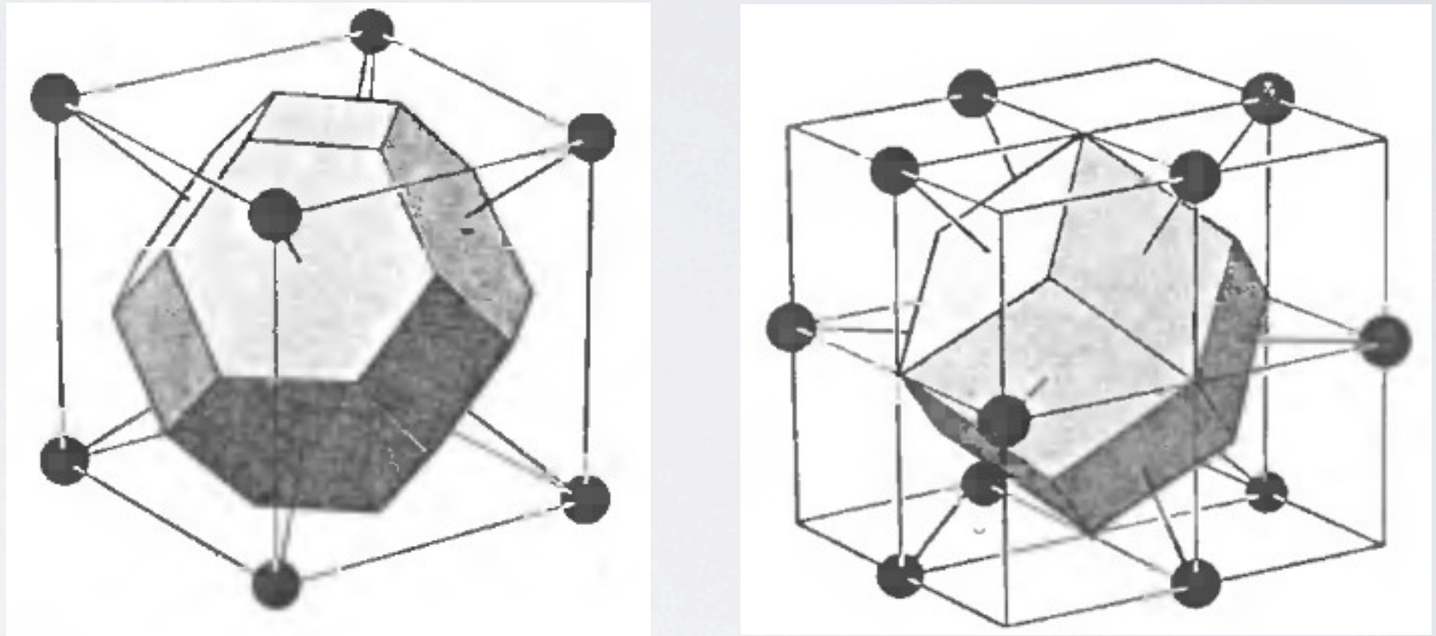
Image source: Wikipedia

WIGNER-SEITZ CELL (CONT.)

- For a given lattice point, the Wigner-Seitz cell is ***the volume of space that is closer to that point than any other in the lattice***

- ***Algorithm for construction***
  - Choose a lattice point
  - Find its nearest neighbors
  - Draw a line from the point to its neighbors
  - Bisect this line with a plane
  - Planes bound the Wigner-Seitz cell

- We will find this same construction useful when we learn about Brillouin Zones



(Left) bcc Wigner-Seitz cell
(Right) fcc Wigner-Seitz cell

- If you ever wind up working in applied math/computer science/topology, a generalization of this concept is frequently found (Voronoi polyhedra) that actually goes all the way back to Descartes!

UNIT CELL VOLUME

- The volume of the unit cell, when occupied by a basis of atoms, will have some bearing upon the physical properties of the crystal.

- The volume of a conventional, cubic unit cell is simply $|\mathbf{a}_1|^3=|\mathbf{a}_2|^3=|\mathbf{a}_3|^3$

- More generally, you can use the lattice vectors to calculate the volume of the unit cell:

$$|\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)| = |\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)| = |\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)|$$

- So far we have only considered the conventional unit cell...
- What about the primitive unit cell?
  - Conventional unit cell for fcc and bcc have 4 and 2 atoms per cell, respectively.
  - What is the volume of the primitive cells for fcc and bcc structures?

EXEMPLARY CRYSTAL STRUCTURES

- Remember, to create an actual crystal, we need to ***assign a basis of atoms to the Bravais lattice***.
- What are some of the more common crystal structures that arise in solid state physics?

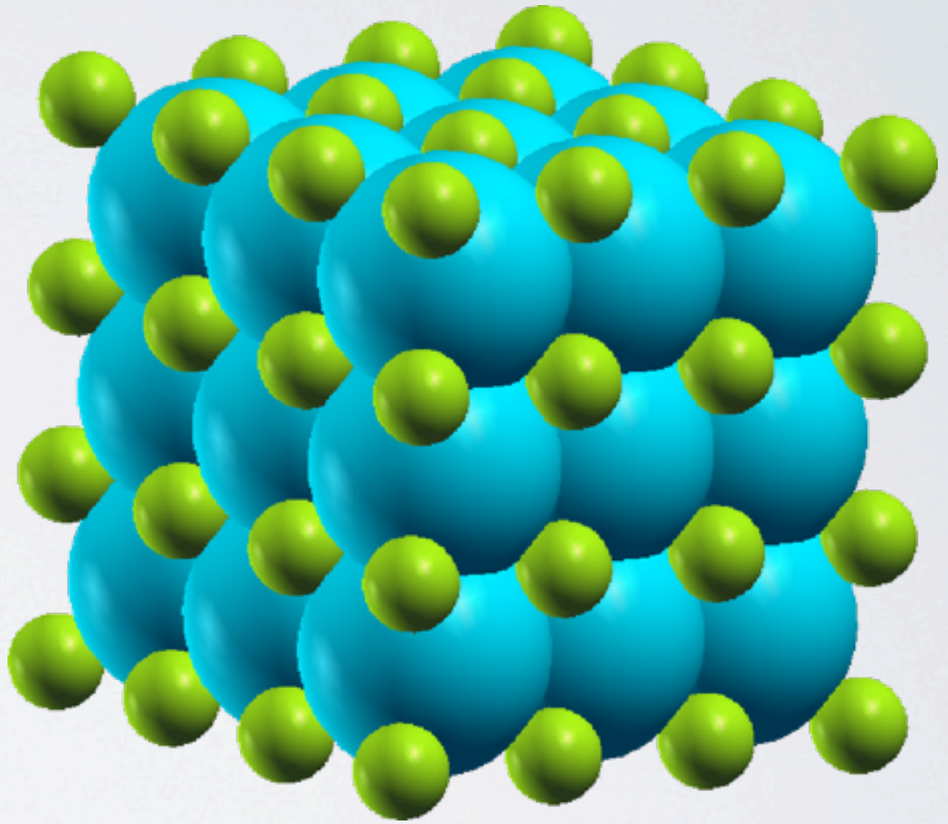
  - ***CsCl:*** simple cubic with a basis of 2 atoms
  - ***NaCl (halite, rock salt)***: fcc lattice with a basis of 2 atoms
  - ***Diamond***: fcc lattice with a basis of 2 atoms of the same species
  - ***ZnS (zincblende)***: fcc lattice with a basis of 2 atoms of different species
  - ***Hexagonal close packed (HCP)***: simple hexagonal lattice with a two atom basis

- Let's look at these individually, in more detail...

CESIUM CHLORIDE

- Simple cubic lattice with a basis of 2 atoms:
  - Green sites are Chlorine
  - Blue sites are Cesium
- Simple choice of basis: (0,0,0) and (a/2,a/2,a/2)
- Each site has ***8 nearest neighbors*** of the opposite species.

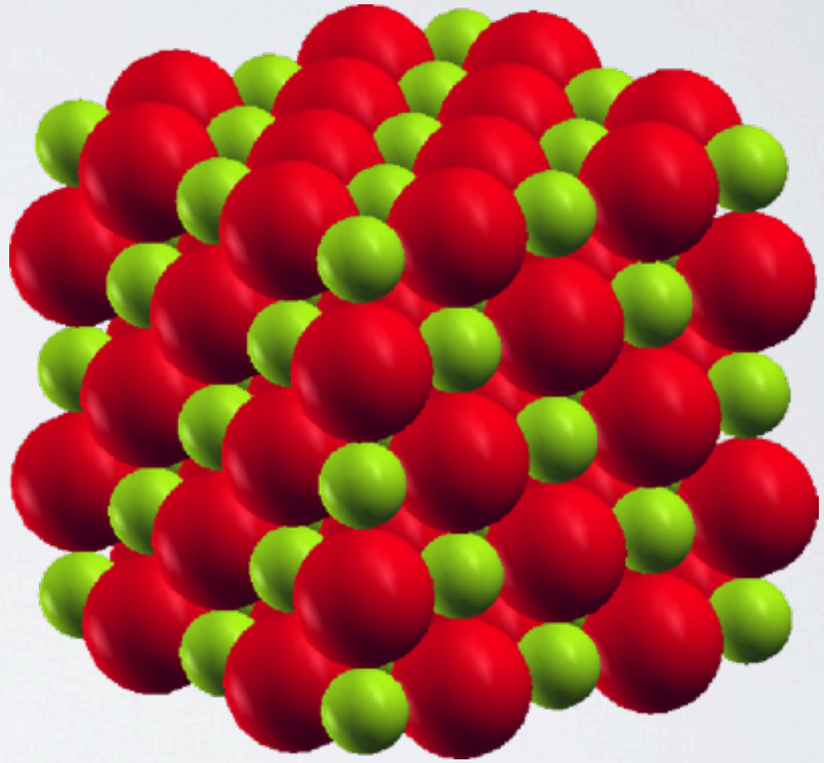
- Alkali halide, so bonding is similar to NaCl, but here the atoms have very different sizes...



SODIUM CHLORIDE

- Face centered cubic lattice with a basis of 2 atoms:
  - Green sites are Chlorine
  - Red sites are Sodium
- Same choice of basis: (0,0,0) and (a/2,a/2,a/2)
- ***Centering*** is different here!
- Each site has ***6 nearest neighbors*** of the opposite species.

- Again an alkali halide, so bonding will be similar, but the atoms have similar 'sizes', so the crystal structure is different.

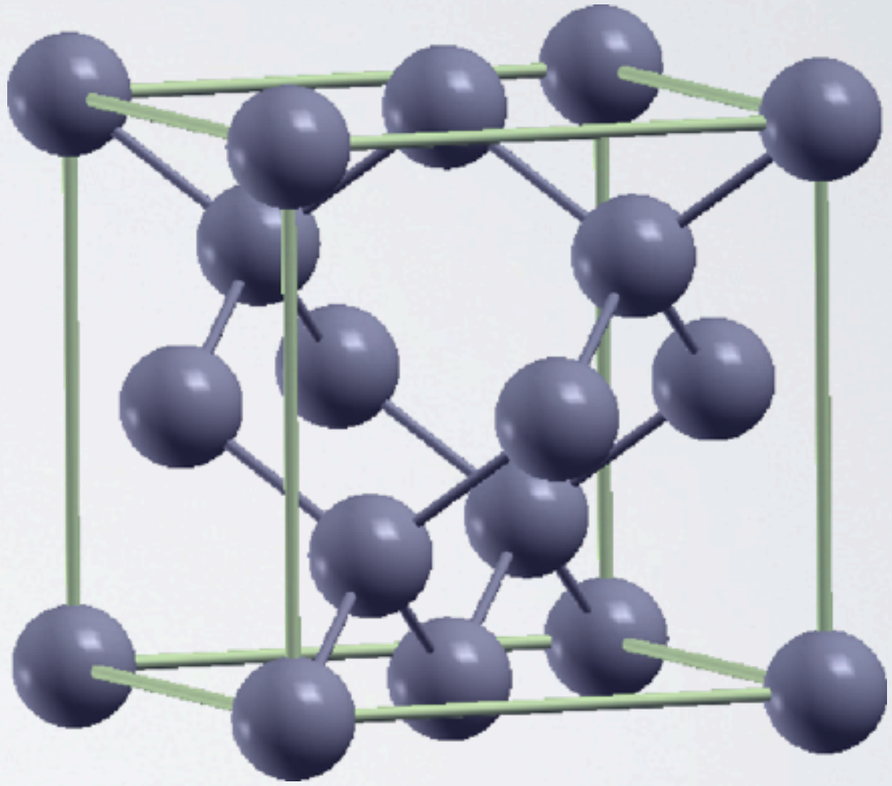


DIAMOND

- Face centered cubic lattice with a basis of 2 atoms of the same species (Carbon for "*diamond*" diamond)

- New choice of basis: (0,0,0) and (a/4,a/4,a/4)
- Centering is different here!
- Each site has 4 nearest neighbors of the ***same*** species.

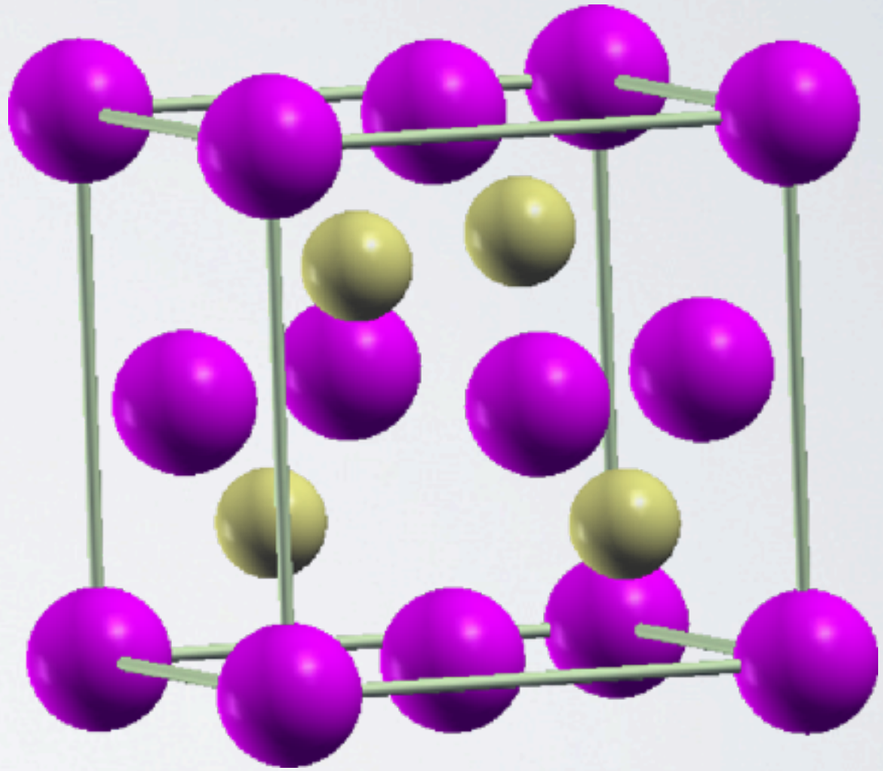
- Diamond structures typically arise in covalently bonded crystals
- Of great technological importance:
  - Silicon solidifies in the diamond crystal structure



ZINCBLENDE

- Face centered cubic lattice with a basis of 2 atoms of the different species (Zinc and Sulfur)
- Same choice of basis: (0,0,0) and (a/4,a/4,a/4)
- Each site has 4 nearest neighbors of the ***opposite*** species.

- Zincblende structures also arise in covalently bonded crystals
- Also of great technological importance:
  - Commonly arises in III-V semiconductors
  - GaAs is a good example



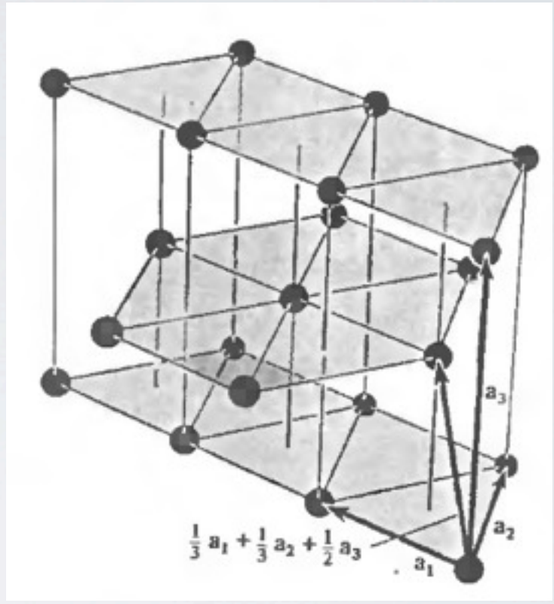
HEXAGONAL CLOSE PACKED (HCP)

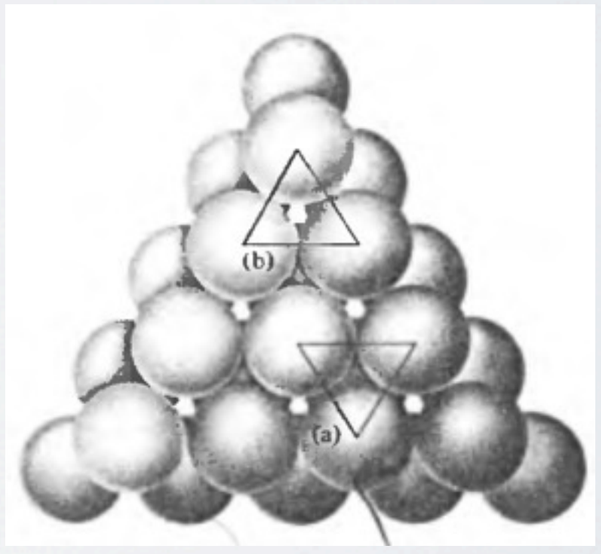
- Simple hexagonal lattice with a basis of 2 atoms
- Think of this as stacking layers of 2D triangular nets
- Basis: (0,0,0) and (a/3,a/3,a/2)

- The name comes from packing hard spheres (bottom)

- 30 elemental solids crystallize in HCP
  - (Mg and Be are the most common)

- Many different types of close-packing arrangements
  - Think of it like close-packing 2D layers...
  - HCP is not Bravais lattice, but FCC close-packing is...





MODERN APPLICATIONS

- The ***topological insulating state*** is a topic of considerable contemporary interest.

- In a conventional ***band insulator***, the electrons in a crystalline solid are immobile throughout the ***entire crystal*** (i.e., even at the surface)

- In a topological insulator, symmetries of the underlying crystal, along with spin-orbit coupling effects give rise to materials where the ***bulk insulates***, but the ***surfaces have electronic states that can participate in conduction***.

- These surface states are very 'exotic':
  - Electron spin is locked perpendicular to its (quasi)-momentum
  - Scattering channels are suppressed by symmetry, so the conduction is ballistic (free of scattering)
  - Anomalous magnetoelectric effect (non-Maxwellian electrodynamics)

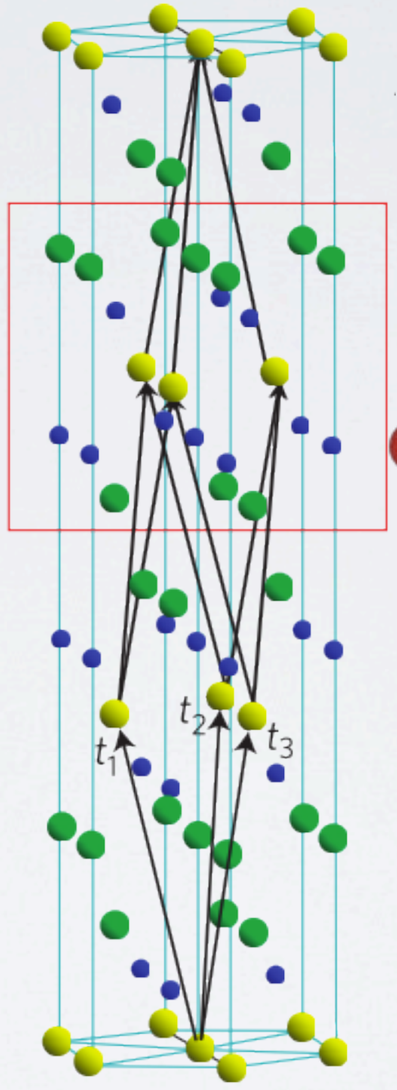
- Some of the associated crystal structures are quite complex...

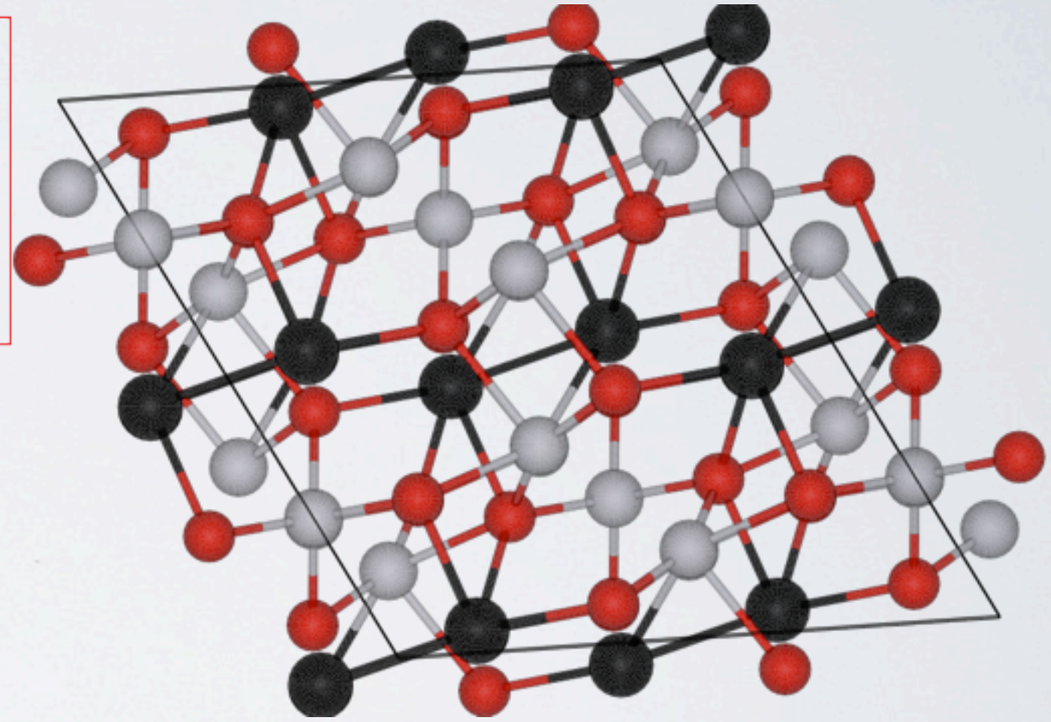
MODERN APPLICATIONS

- On the left is Bi_2Se_3, a confirmed topological insulator
  - Rhombohedral Bravais lattice

- On the right is $Tl_2Hg_3Te_4$, a potential topological insulator
  - Monoclinic Bravais lattice

- I am studying the latter, trying to figure out whether or not this state will arise in this particular material





CONCLUSIONS

- Take home points from today's lecture:
  - There are ***14 distinct Bravais lattices in 3D***.
  - Each lattice is ***characterized by 3 lattice vectors*** (3 magnitudes, 3 angles)
  - Primitive cell can be constructed using ***Wigner-Seitz method***

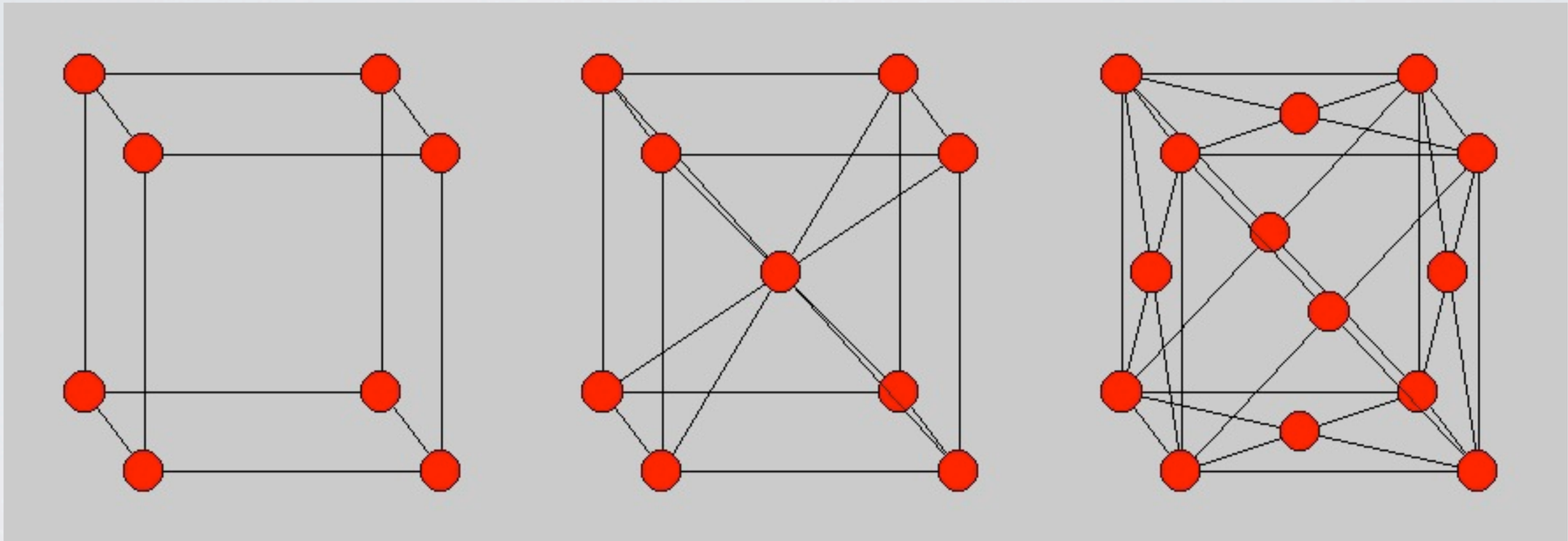
- In Monday's lecture, we will discuss:
  - What type of ***experimental probes*** exist for characterizing crystalline solids?
  - What is a ***reciprocal lattice*** and what is its relationship to the lattices we have already discussed?
  - What is a ***Brillouin Zone***, and why is it theoretically useful?

- ***Any questions?***

- ***Before leaving, take out a piece of paper - here is a 5 minute quiz.***

QUIZ

- *Consider the simple cubic, face centered cubic, and body centered cubic lattices.*



- *Assuming each lattice site is occupied by a basis consisting of a single sphere at (0,0,0), with a radius such that it is touching its nearest neighbor, what percentage of the conventional unit cell is filled by spheres?*