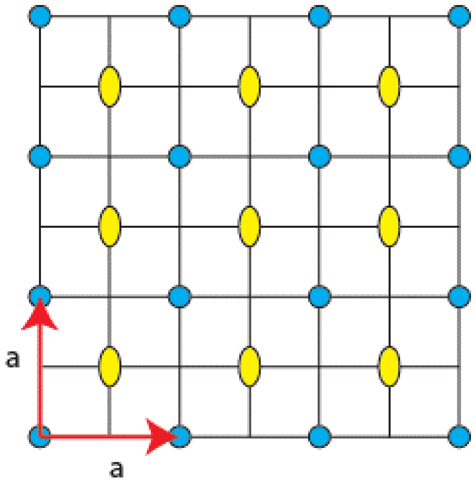
Outline:

- **Review key concepts from last lecture (lattice + basis = unit cell)**
- **Bravais lattices**
- **Important crystal structures**
- **Intro to miller indices**

Review (example with square lattice)



Lattice: square, with chosen primitive translation vectors $u_1 a\hat{x}, u_2 a\hat{y}$ (u_1 and u_2 are integers); remember, the lattice is a mathematical mesh of points on space

Basis: blue circle (located at (0,0)) + yellow oval (located at (a/2,a/2)); basis coordinates are found by identifying repeating unit cell, setting one corner of the cell as (0,0), and finding the fractional coordinate of the other atom(s) in the basis in terms of the chosen primitive translation vectors

Unit cell=lattice+basis; repeating unit in crystal

Last lecture we discussed the 'primitive cell' which is a property of the **lattice** (mathematical construct). The **unit cell** is a building block of a **crystal**

Crystal systems (lattices)

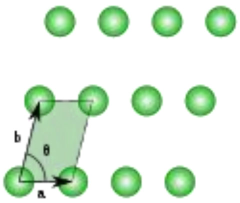
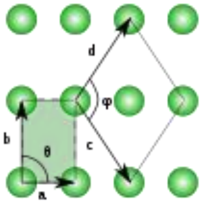
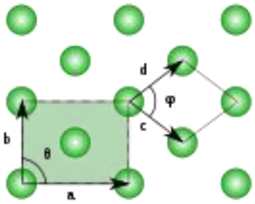
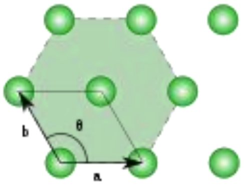
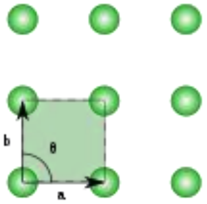
In two dimensions there are **5** special lattice types, defined by the symmetry operations which render them invariant. In 3 dimensions, there are **14** lattice types. These are referred to as Bravais lattices. All of these are primitive lattices, but sometimes they have a 'conventional' unit cell with is more convenient, but not primitive

Demo: 14 3D Bravais lattices

2 dimensions (draw on board):

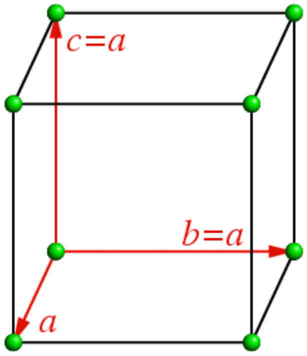
- Going from right to left, there are fewer symmetries

- Body-centered-rectangular (3): note distinction between **conventional cell** (two atoms per cell) and **primitive cell** (diamond with translation vectors **c** and **d**; one atom per cell). The conventional cell is often used for convenience (it is easier to work with orthogonal translation vectors), but the fact that a primitive cell **can** be constructed allows the body-centered rectangular cell to be counted as a Bravais lattice
- To reiterate, all of the 5+14 crystal systems discussed here represent only the possible lattice groups; Once we add a basis, we can describe the microscopic structure of most inorganic solids

 1	 2  3	 4	 5
$\|a\| \neq \|b\|,\ \theta \neq 90°$	$\|a\| \neq \|b\|,\ \theta = 90°$ $\|c\| = \|d\|,\ \varphi \neq 90°$	$\|a\| = \|b\|,\ \theta = 120°$	$\|a\| = \|b\|,\ \theta = 90°$
m	o	h	t

3 dimensions:

- Black arrows in images below show the **primitive translation vectors** in cases where the conventional cell differs from the primitive one
- Explain what $a_{1,2,3}$ and $\alpha_{12}, \alpha_{23}, \alpha_{31}$ are
- In class: make table with Bravais lattice type, parameters, and examples
- In class example: how many atoms are in conventional FCC lattice?
  - 8 corners (each shared among 8 unit cells)=1
  - 6 faces (each shared among 2 unit cells)=3
  - 1+3=4
- In-class example: find primitive translation vectors for BCC lattice (they are shown in the table below)



If lattice vectors in the conventional cell are given by $(a\hat{x}, a\hat{y}, a\hat{z})$ with the x,y,z direction given in the figure above (y is to the right and z is up), the primitive lattice vectors are $[\frac{a}{2}(\hat{x}+\hat{y}-\hat{z}), \frac{a}{2}(\hat{x}-\hat{y}+\hat{z}), \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z})])$. If x, y, z directions defined differently, the primitive lattice vectors will have different (but mathematically equivalent) expressions. Thus, please indicate your coordinate system on your homework/exams.

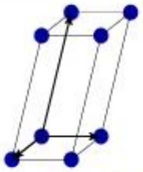
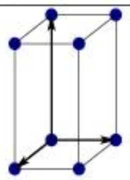
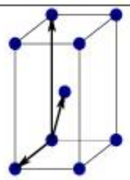
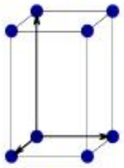
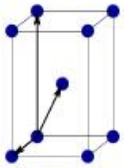
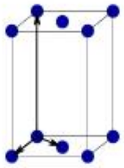
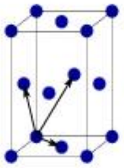
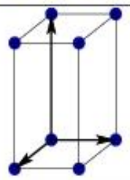
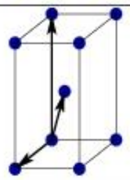
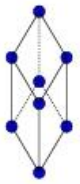
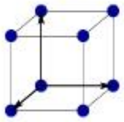
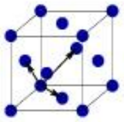
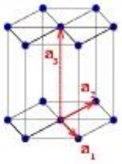
Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
Orthorhombic	$a_1 \neq a_2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

Examples of each one:

Hexagonal	Many metals including cobalt and zinc have a variation of the hexagonal crystal structure called ‘hexagonal close packed’
Simple Cubic	The only element which is simple cubic is polonium

Body Centered Cubic	Many metals including lithium, sodium, potassium, chromium
Face Centered Cubic	Many metals including Copper, Silver, Gold Platinum
Trigonal	Quartz, calcite
Tetragonal	Nonlinear crystal inside green laser pointer
Body centered tetragonal	
Orthorhombic	
Body Centered Orthorhombic	
Base Centered Orthorhombic	
Face Centered Orthorhombic	
Monoclinic	
Body centered Monoclinic	
Triclinic	

Resource for 3D crystal structures you can manipulate:
http://www.chemtube3d.com/solidstate/_table.htm

Common crystal structures

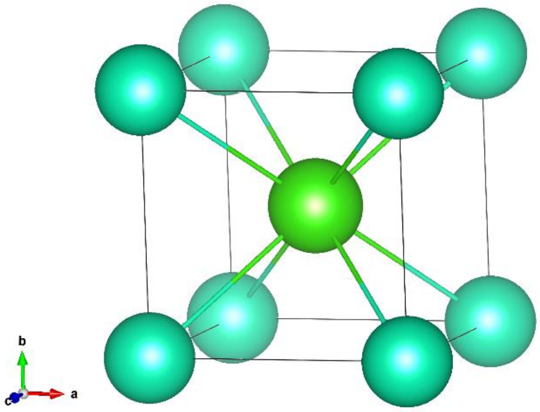
Start with two building blocks: **close-packed triangular lattice** or **cube**

Cube:

CsCl

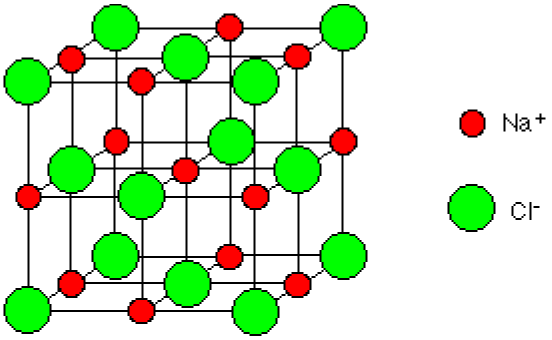
What is basis? (one Cs ion at (0,0,0) and one Cl ion at (1/2, ½, ½)

What is lattice type? (simple cubic, with 2 atom basis)



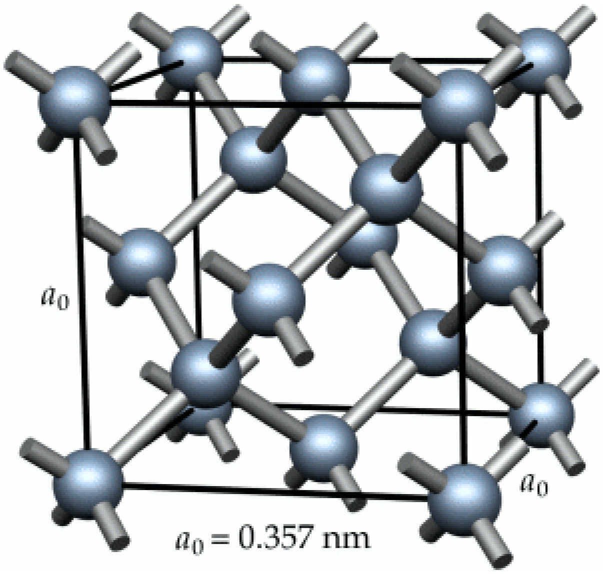
(sort of like BCC except with different atom at center)

NaCl



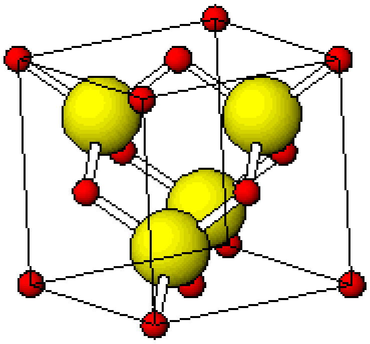
(two interpenetrating FCC lattices)

Diamond



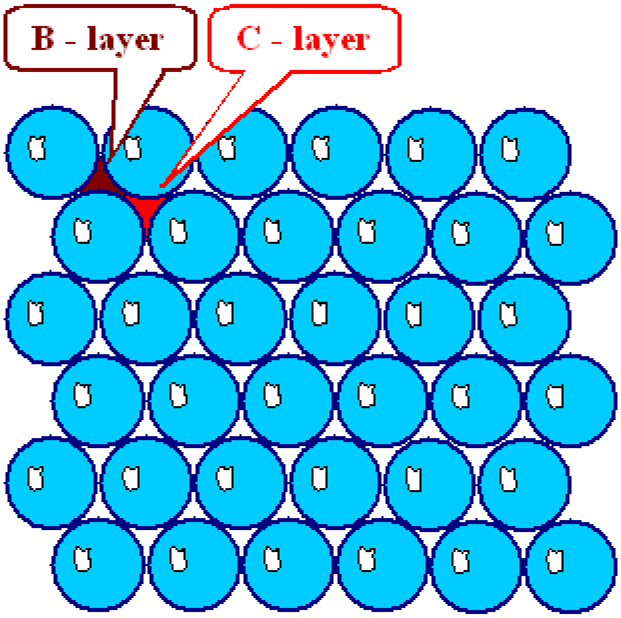
(FCC with additional atoms at (1/4, ¼,1/4), (3/4, ¾, 1/4), (3/4,1/4,3/4),(1/4,3/4,3/4); this is a very important crystal structure in science and engineering because silicon takes on this structure)

Zincblende



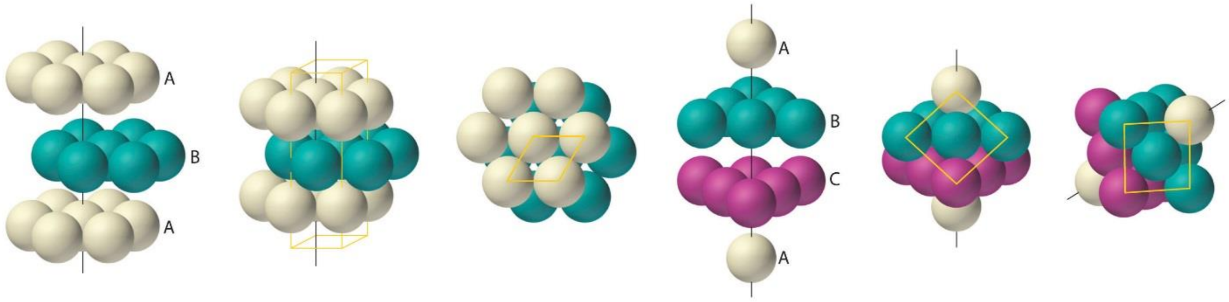
(similar to diamond lattice except with different atoms in the interior)

Hexagonal lattice:



When hexagonal lattices are stacked on top of one another, this is the procedure:

- First layer: Centers of circles = **A** sites
- 2nd layer: two choices for 2nd layer--circles centered on right-side up triangles (B) or upside-down triangles (C); lets choose **B**
- 3rd layer: two choices for 3rd layer relative to first layer—**A or C**
- ABABABAB… stacking: hexagonal-close packed (HCP)
- ABCABCABC… stacking: face centered cubic



(a) Hexagonal close-packed (hcp) **(b) Cubic close-packed (ccp)**

Packing Fraction (for homework)

Diffraction equation and crystallographic planes

Demo: diffraction gratings + laser; CD+laser

Diffraction is the general way that one learns about a material's repeating structure. It is one of the most useful tools in solid state physics and in applications of solid state physics and the formalism surrounding it (especially the concept of reciprocal lattice) is the most important thing you will learn in this class.

What a diffraction grating is:

- A sheet with lines scratch in it
- The spacing between lines is comparable to the wavelength of light used
- Bragg's law: $2d sin\theta = n\lambda$ (will derive in the next class)

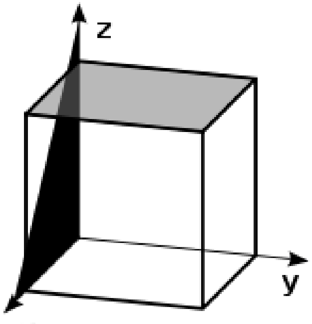
In a 3D crystal lattice, d is the spacing between crystallographic planes. There are many ways to slice a given crystal structure into planes, and the system of **miller indices** is how we describe each plane (demonstrate a few on simple cubic structure).

The process of finding miller indices:

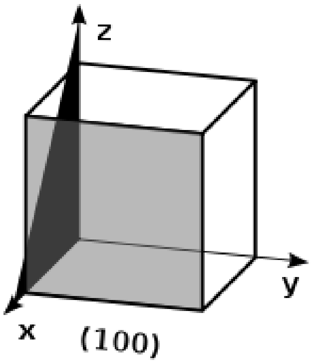
1. Find the intercepts on the axes in terms of the lattice constants a_1, a_2, a_3; Integer or fractional intercepts are fine
2. Take the reciprocals of these numbers and reduce to 3 smallest integers
3. Express result as 3 numbers in parentheses, usually no commas (hkl)

Below: examples for cubic lattice

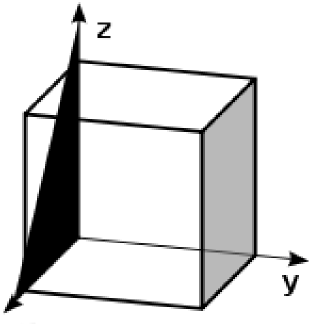
(in class: also give example of (200) plane where intercepts are at (1/2, 0,0)



(001)



(100)



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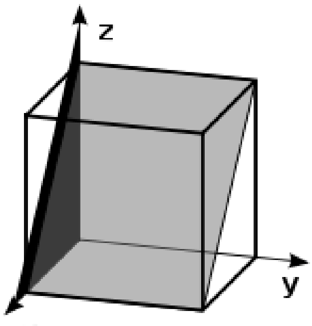

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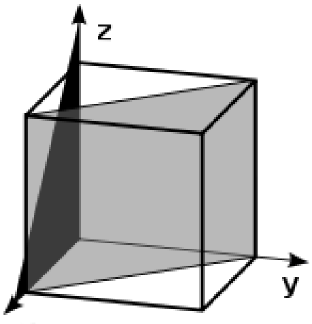

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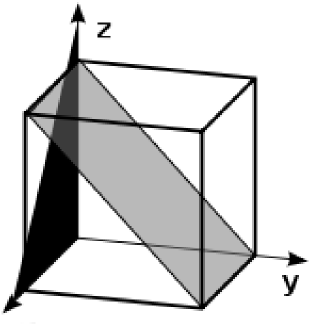

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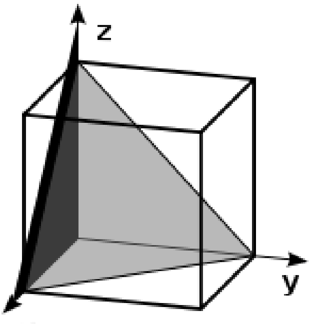

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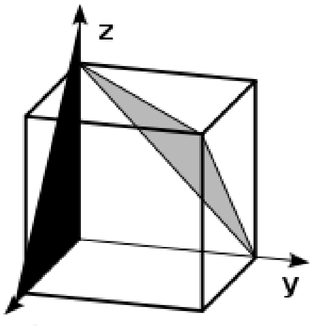

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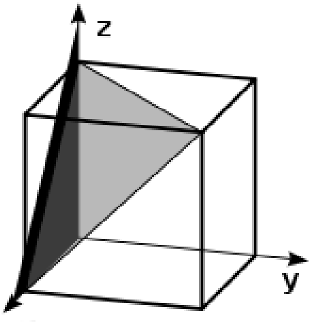

$(\bar{1}\bar{1}1)$

More properties of miller indices:

- If intercept is negative, place bar above the index (e.g. center and right of bottom row above)
- Often, there will be planes with equivalent symmetry (e.g. 001 100, 010 for cubic system) these are indicated with curly brackets, e.g. {100} set of planes encompasses the entire top row above, as well as (-100),(0-10),etc
- Sometimes planes are parallel but inequivalent, e.g. (100) and (200) (the latter cuts x-axis at (1/2, 0, 0)

  Relationship between Miller indices and d in Bragg equation: 3D crystal structure contains repeating planes and the distance between these repeating planes sets d. The miller index notation/procedure is a mechanism for slicing the 3D crystal structure into planes