

## Overview of the course

In this course we will try to understand the sometimes strange behavior of solids (as opposed to liquids, gases, and plasmas) that leads to modern electronics with their transistors, diodes, and LED's.

In particular, we will try to see why some materials (metals) are good but not perfect conductors of both heat and electricity, others are insulators, and a few others are the so-called semiconductors.

We'll see that temperature plays an important role in electrical properties of material, and so we'll have to look at heat before we look at electricity in solid materials.

In order to understand heat energy in solids, we will have to look at how solids are constructed.

The first section of the course deals with the physical construction of solids and the **lattice**.

The second section of the course deals with **heat**. We know that heat energy in gases is actually the kinetic energy of the molecules: the higher the temperature the more kinetic energy of the molecules. But in solids, the molecules are tied together and so can't have the same kind of energy as free molecules. We'll see where the heat energy in a solid is, and how it moves through the solid (heat conduction).

The third section of the course deals with **electrical conduction** in metals and insulators, and how temperature plays a part.

The fourth section of the course deals with **semiconductors** and their use in transistors, diodes, and LED's.

In dealing with the atoms of the solid, we will have to employ some basic quantum mechanics. Recall that in Physics III we saw that we have a **wave-particle duality** for light – and for electrons! We will have to employ this wave-particle duality in this course. For light, the photon (particle) energy was related to the electromagnetic wave by  $E = hf = \hbar\omega$  (where  $\hbar = h/2\pi$  and  $\omega = 2\pi f$ ) and the momentum was related by  $\lambda = h/p$  (or  $p = \hbar k$  where  $k = 2\pi/\lambda$ . Note: in 3-D,  $\mathbf{k}$  will be a vector just like  $\mathbf{p}$ , the momentum). We will run into a similar wave-particle duality for oscillations in a solid that will introduce the concept of a “particle” of vibration called a phonon. This concept will be used in the electrical and semiconductor sections that follow.

### Review of terms:

|  |   |
|--|---|
| $E$ = energy (MKS unit is Joule)               | $h$ = Planck's constant = $6.63 \times 10^{-34}$ J-s; |
| $f$ = frequency in cycles/sec;                 | $\omega$ = angular frequency in radians/sec;          |
| $\mathbf{p}$ = linear momentum = $m\mathbf{v}$ | $\lambda$ = wavelength                                |

# Crystal Structure

**1. Atoms are bound together in a solid.** Due to the nature of the forces that bind the atoms together (and hence due to the energies involved), the atoms sometime show a high degree of symmetry in their alignment. An ideal crystal has this symmetry perfectly.

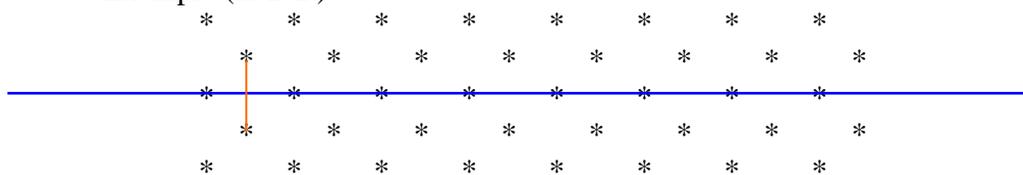
**2. Crystal, lattice, and basis:** Sometimes, though, the symmetry is based on molecules instead of individual atoms. To deal with this, we use the following terminology:

An ideal **crystal** is composed of a perfectly symmetric series of **lattice points**, and associated with each lattice point is a **basis** which consists of an atom or a set of atoms.

**3. Symmetries:** There are different standard types of lattices based on the different types of symmetries that are possible.

a) **reflection** symmetry: If the lattice looks the same above and below a plane (looks like a mirror image), then the lattice has a reflection symmetry.

Example (in 2-D):



Counter-example (in 2-D):



b) **rotation** symmetries: If the lattice looks the same when you rotate through a certain angle, then that lattice has that particular rotation symmetry. All lattices, of course, have a  $360^\circ$  (or  $2\pi$  radians) symmetry. All lattices also have a  $180^\circ$  (or  $\pi$  radians) symmetry. This is due to the repetitive nature of a lattice: if there is a lattice point in front of a certain lattice point, there is another lattice point behind that certain lattice point. If there is lattice point at a certain angle from that lattice point, then there will be another lattice point  $180^\circ$  from that angle from that certain lattice point. Try to see this in both of the above examples in part a.

If a lattice has **ONLY** these  $360^\circ$  and  $180^\circ$  symmetries, then it is called an **oblique** lattice.

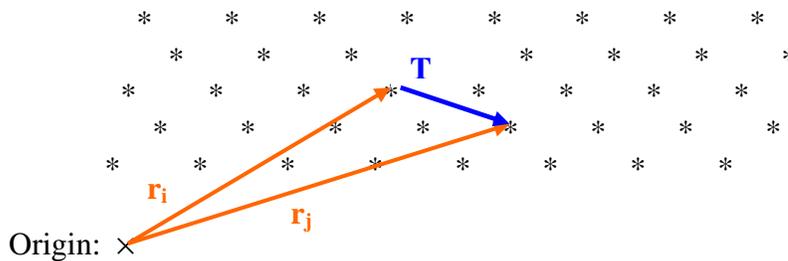
Lattices can have other rotational symmetries in addition to  $360^\circ$  and  $180^\circ$ . If we confine ourselves to 2-D lattices (easier to see and draw), we can get some kind of experience in identifying possible lattice symmetries. Can you draw/visualize a lattice with  $90^\circ$  ( $2\pi/4$ ) rotational symmetry? A **square lattice** has this. Can you visualize a lattice with  $120^\circ$  ( $2\pi/3$ ) rotational symmetry? A **hexagonal lattice** has this. Also, when you draw it, you'll see it also has a  $60^\circ$  ( $2\pi/6$ ) symmetry. Can you visualize a pentagonal symmetry ( $72^\circ$  or  $2\pi/5$ ) symmetry? When you try to do this, you will see that you do NOT create a lattice that is repeatable! Are there any more "special" types of lattices you can see? Yes, a **rectangular lattice**. It does NOT have a  $90^\circ$  symmetry, but it does have a reflection symmetry. There is also a **centered rectangular lattice** which also has reflection

symmetry. Thus, we have identified **5 types of 2-D lattices**: the general **oblique** lattice that does NOT have reflection or anything beyond  $360^\circ$  and  $180^\circ$  rotational symmetries; the **square** lattice, the **hexagonal** lattice, the **rectangular** lattice, and the **centered rectangular** lattice.

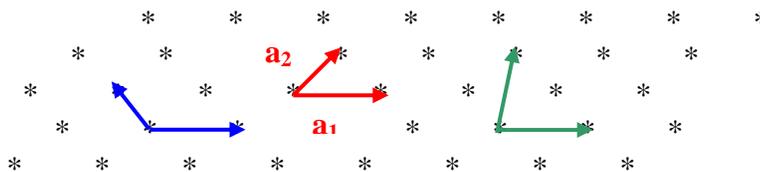
#### 4. Translation Vectors ( $\mathbf{T}$ ) and lattice vectors ( $\mathbf{a}_i$ )

In order to make the lattice type identifications more mathematical, we employ the idea of a **translation vector**,  $\mathbf{T}$ . If you are at a lattice point that has a location  $\mathbf{r}_i$ , by adding the translation vector,  $\mathbf{T}$ , you end up at another lattice point,  $\mathbf{r}_j$ :

$$\mathbf{r}_i + \mathbf{T} = \mathbf{r}_j, \text{ or equivalently } \mathbf{T} = \mathbf{r}_j - \mathbf{r}_i$$



Following this idea, we can see that we can define a translation vector,  $\mathbf{T}$ , in terms of integer values of (in 2-D) two basic translation vectors, called **primitive** translation vectors.



Example: Note that either the **red or the blue pair of vectors can** be used so that any lattice point can be reached from any other by using only integer values of  $\mathbf{a}_1$  and  $\mathbf{a}_2$ .

Counter-example: but **the green pair can NOT** reach all lattice points in the same way.

$$\mathbf{T} = n\mathbf{a}_1 + m\mathbf{a}_2, \text{ where } n \text{ and } m \text{ are integers.}$$

#### 5. 2-D Lattice Types – revisited.

For a **square lattice**, we can see that  $|\mathbf{a}_1| = |\mathbf{a}_2|$ , and that the angle,  $\phi$ , between  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , is  $90^\circ$ .

For a **hexagonal lattice**,  $|\mathbf{a}_1| = |\mathbf{a}_2|$ , and that the angle,  $\phi$ , between  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , is  $120^\circ$  (or we could choose  $60^\circ$ )

For a **rectangular lattice**,  $|\mathbf{a}_1| \neq |\mathbf{a}_2|$ , and that the angle,  $\phi$ , between  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , is  $90^\circ$ .

For a **centered rectangular lattice**,  $|\mathbf{a}_1| \neq |\mathbf{a}_2|$ , and that the angle,  $\phi$ , between  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , is less than (or greater than)  $90^\circ$ .

For an **oblique** lattice there are no special relations. See above for an example.

*Homework problem #1* has you draw an example of each of these five types.

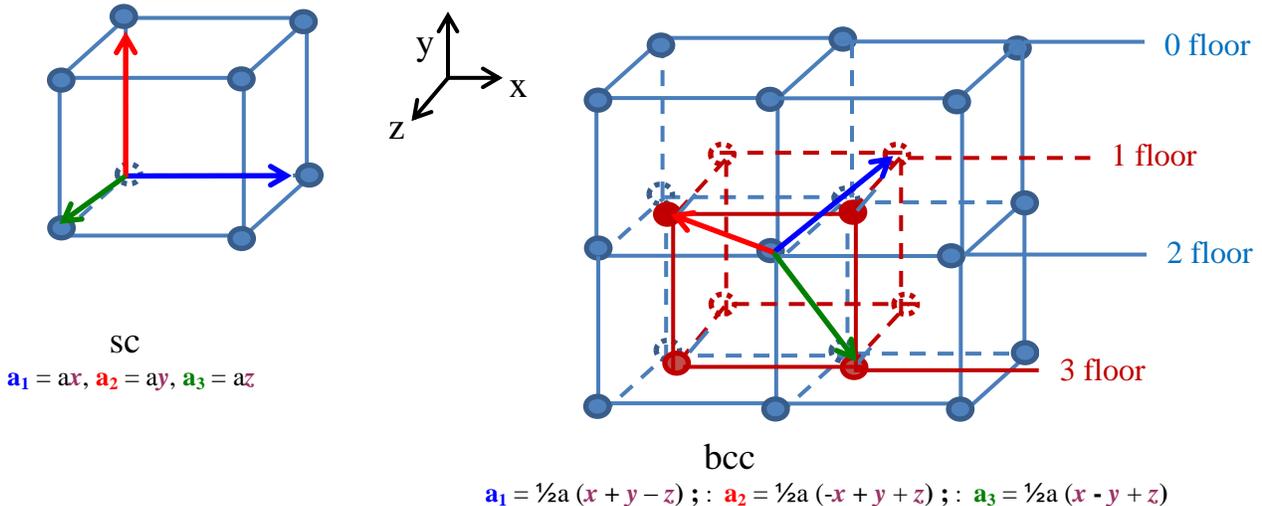
## 6. 3-D Lattice Types

There are **14 basic lattice types in 3-D**, but we will only be concerned about a few. Sometimes the 3-D lattice types are better described in terms of non-primitive descriptions, but we should always remember that we will need primitive lattice vectors to work fully with the mathematical descriptions.

a) The easiest 3-D lattice to work with is the simple cubic lattice (**sc**) which has lattice points on all the corners of a cube. It is just the 3-D extension of the 2-D square lattice. If we align the  $x, y, z$  axes with the cube, we get primitive lattice vectors:  $\mathbf{a}_1 = a\mathbf{x}$ ,  $\mathbf{a}_2 = a\mathbf{y}$ ,  $\mathbf{a}_3 = a\mathbf{z}$ .

In the figure below on the right for the bcc lattice, dotted lines and blue dotted circles  $\odot$  are hidden in the back, solid lines and solid circles  $\bullet$  are in the front,  $\odot$  points are body centered points between back and front rows; solid red points  $\bullet$  are body centered points on top of the front row of  $\bullet$ .

For the bcc lattice, notice that the blue dots can be seen as the corner dots with the red dots as the body centered dots; but also the red dots can be seen as the corner dots of the lattice with the blue dots as the body centered dots.



b) A second 3-D lattice that has a nice 3-D extension of a 2-D lattice is the body centered cubic lattice (**bcc**) – above on the right. In this lattice, in addition to having lattice points at all the corners of a cube, there is a **lattice point right in the middle** of the volume of the cube. A convenient way of identifying primitive lattice vectors is to start at a lattice point at a corner of the cube and choose lattice vectors to three of the nearest center lattice points. This gives:

$$\mathbf{a}_1 = \frac{1}{2}a(x + y - z) ; ; \mathbf{a}_2 = \frac{1}{2}a(-x + y + z) ; ; \mathbf{a}_3 = \frac{1}{2}a(x - y + z) .$$

Note: we could have chosen to make  $\mathbf{a}_1 = \frac{1}{2}a(x + y + z)$ , but then we would have various combinations of minus signs in the other two primitive lattice vectors,  $\mathbf{a}_2$  and  $\mathbf{a}_3$ . The above choice has a very nice symmetry to it.

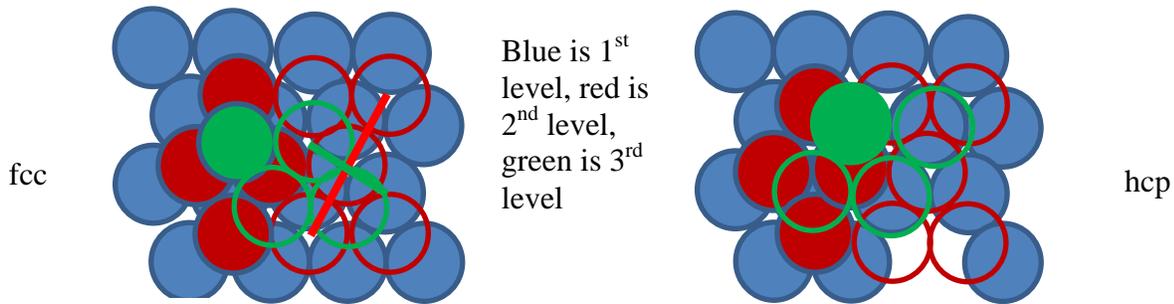
Note that in the sc lattice each lattice point has six nearest neighbors, one above and one below, one on the left and one on the right, one in and one out. In the bcc lattice each lattice point has eight nearest neighbors since the body centered lattice point has the eight corner lattice points.

c) Another 3-D lattice is one based on the 2-D hexagonal lattice. Actually **two** of the 3-D lattices are based on the 2-D hexagonal lattice: the face centered cubic (**fcc**) and the hexagonal close packed (**hcp**). These two lattices have the hexagonal structure in 2-D, but have **different stacking's** for the planes that fit on top to create the 3-D lattice.

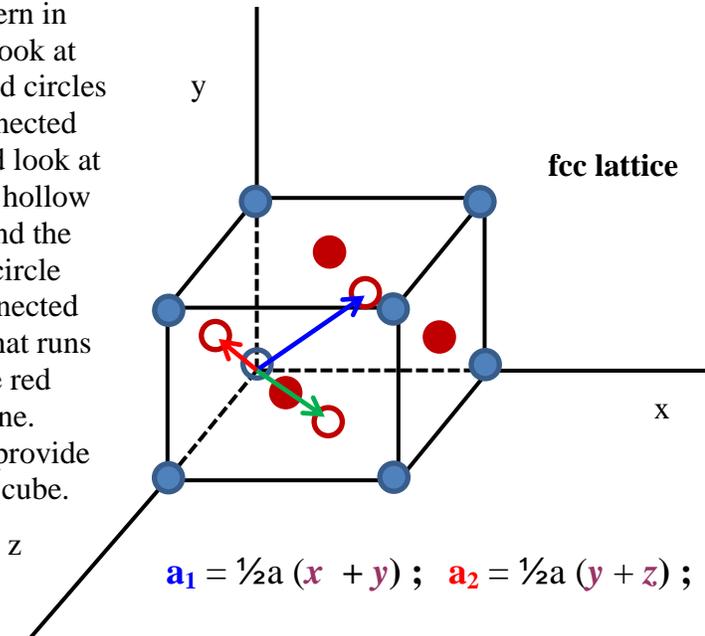
The fcc structure has a cubic structure with lattice points at the corners of the lattice like the sc lattice, but in addition it has lattice points in the **center of all six faces** (sides) of the cube. It does NOT have a lattice point in the middle of the cube like a bcc lattice does. A convenient way of identifying primitive lattice vectors is to start at a corner of the lattice and choose lattice vectors to three of the **nearest face centered** lattice points. For the **fcc**, a good (symmetric) choice of primitive lattice vectors is:

$$\mathbf{a}_1 = \frac{1}{2}a (\mathbf{x} + \mathbf{y}) ; \quad \mathbf{a}_2 = \frac{1}{2}a (\mathbf{y} + \mathbf{z}) ; \quad \mathbf{a}_3 = \frac{1}{2}a (\mathbf{x} + \mathbf{z}) .$$

On the **left** below, an **fcc** lattice, is a blue hexagonal plane, with a red hexagonal plan on top, and with a third green hexagonal plane that fits above holes in both the first (blue) and second (red) planes. On the **right**, an **hcp** lattice, the third (green) plane fits directly above the atoms in the blue plane (hcp).



To see the fcc pattern in the hex structure, look at the three hollow red circles (middle level) connected by the red line, and look at the top right green hollow circle (top level) and the 3<sup>rd</sup> row right blue circle (bottom level) connected by the green line that runs through the middle red circle of the first line. These five circles provide one side of the fcc cube.

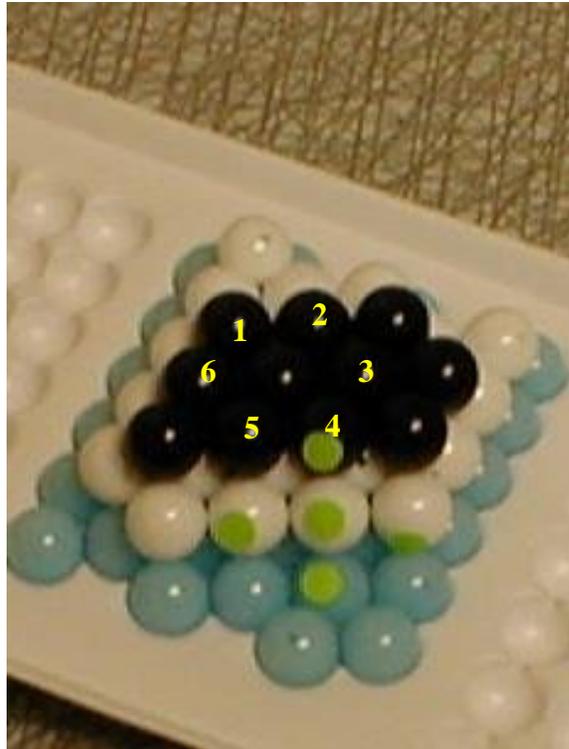


In the fcc lattice each corner lattice point has 12 nearest neighbor lattice points: four on the four face diagonals in one plane, four face diagonals in the plane above, and four face diagonals in the plane below. Viewed from the hex plane, each lattice points has six nearest neighbors in the hex plane, and three nearest neighbors above and three below for a total of 12.

$$\mathbf{a}_1 = \frac{1}{2}a (\mathbf{x} + \mathbf{y}) ; \quad \mathbf{a}_2 = \frac{1}{2}a (\mathbf{y} + \mathbf{z}) ; \quad \mathbf{a}_3 = \frac{1}{2}a (\mathbf{x} + \mathbf{z})$$

The hollow red dots are the face centered dots on the back three sides of the cube, while the filled red dots are the face centered dots on the front three sides of the cube.

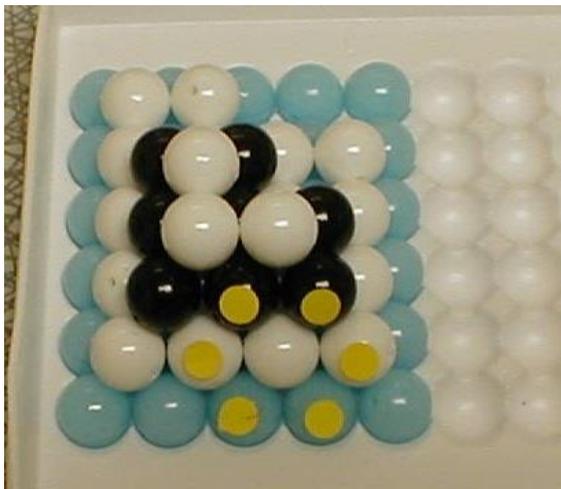
As with the bcc cube, the red dots above appear to be the face centered dots on the blue cube, but they can also be seen as the corner dots of a red cube with the blue dots as the face centered dots.



The image on the left shows four hex planes: the bottom blue, the white, the black, and the top blue. The green dots on the five spheres show one face of the fcc structure: the three white spheres with the green dots are touching and in line; the blue, white, and black spheres with the green dots are also touching along a straight line, and that line is perpendicular to the first line with the white spheres. Note that the four corner spheres on the face do not touch.

The image on the right shows the black hex plane – each sphere touches six on its sides. Note that in the hex planes above and below the white hex plane, the black and blue marbles are not directly above one another.

The two images below show the hcp structure. The horizontal plane is square with the four atoms on a square touching at the sides, but the six marbles in yellow show the hex pattern in a different plane. In that hex plane (plane with all six yellow dotted marbles) the black plane marbles sit directly above the blue plane marbles.





In the images above, you see the bcc structure. The white plane marbles do not touch on the side. The blue plane marbles sit and touch the four white marbles in the square below, and they touch the four black marbles in the plane above. Any one blue marble does not touch another blue marble but it does touch all four white and all four black corner marbles.

## 7. Volumes in 3-D lattices

a) Let's consider the volumes associated with the above three types of 3-D lattices.

a1) The easiest to see is the **sc**. It should be easy to see that each lattice point has a volume of  $a^3$  associated with it. (To see this, simply image each lattice point goes forward half way to the next lattice point. This gives  $+1/2a$  forward and backward in each of the three directions, giving a volume of  $a^3$  for each lattice point. Alternatively, each cube can be seen to have a corner on a lattice point. Since a corner lattice point is actually part of 8 different cubes, each corner lattice point contributes  $(1/8)$  of a point to each cube. But since each cube touches 8 lattice points (4 points on a square at the bottom and 4 points on a square at the top), the number of lattice points per cube is 8 lattice points times  $(1/8)$  per lattice point giving 1 lattice point per cube, or 1 lattice point per volume of  $a^3$ .

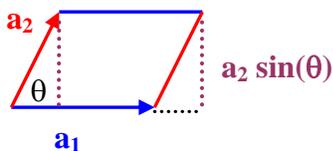
a2) For the **bcc**, we can visualize the sc cube with an additional lattice point in the middle. Thus a volume of  $a^3$  contains two lattice points, and hence the volume associated with each lattice point is  $1/2 a^3$ .

a3) For the **fcc**, we can again visualize the sc cube with additional lattice points in the middle of each of the six faces. Since each of the face lattice points actually touches two cubes, each of these six lattice points count only  $1/2$  for each cube. This gives 1 lattice point from the simple cube plus  $6 * 1/2$  for each of the face centers giving a total of 4 lattice points per cube, or a volume per lattice point of  $1/4 a^3$ .

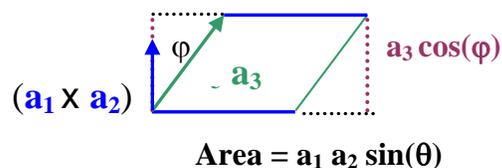
An **alternative way** of getting the volume associated with each lattice point is using the primitive lattice vectors. Since the area defined by a pair of 2-D distance vectors is the length of each times the sine of the angle between the two (area of a parallelogram), the magnitude of the cross product of the two vectors should give the area with a direction perpendicular to both ( $\mathbf{a}_1 \times \mathbf{a}_2$ ). To get the volume, the length that is perpendicular to this area should be multiplied by the area. But this is just the dot (scalar) product of the third vector with the previous area vector:

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

Top view showing area



Side view showing volume



## 8. Hole sizes in the 3-D lattices

If we assume atoms have spherical shapes and the volumes are basically box shapes (to completely fill up the space), there will always be empty places in the volume. To find out where and how big these empty spaces are, we need to first find out where the atoms touch.

a) In the simple cubic (**sc**) lattice, the nearest atoms touch along the cube edges. This means that if there is an atom at one lattice point, the next nearest atom is a distance “a” away. Since the atoms touch along this distance,  $a = 2r$  where  $r$  is the radius of the lattice atom. It is easy to see that the biggest empty space will be right in the middle of the cube. The full diagonal of the cube is:  $d = \sqrt{[a^2 + a^2 + a^2]} = \sqrt{3} * a$ . The space actually taken up is  $2r$ . Therefore the biggest sphere (atom) that could fit in that hole without further spreading out the lattice would have a diameter of  $\sqrt{3}*a - 2r$  (but  $2r = a$ ) so the biggest sphere would have a diameter of  $(\sqrt{3}-1)*a$ , or it would have a radius of  $(\sqrt{3}-1)*r$ . It is one of the homework problems to determine where the lattice atoms touch in a bcc and in an fcc lattice. It is also one of the homework problems to determine the diameter of a sphere that would fit in the biggest hole in each of these three lattices (*Problems 2, 3, and 4*).

b) How much space is actually being used by the atoms and how much space is “empty”? We use the concept of **packing fraction** to quantify this. The packing fraction is simply the volume of the atoms divided by the total volume of the lattice. For a simple cubic (**sc**) lattice with atoms only at the lattice points (monatomic lattice), the packing fraction would be:  $pf = (4/3)\pi r^3 / a^3$  but since  $a = 2r$  (atoms touch along the edges), we get  $pf = (4/3)\pi r^3 / (2r)^3 = 4\pi / 3*8 = \pi/6 = .524$ . Again, it is a homework assignment (*Problem 5*) to determine the packing fractions for bcc and fcc lattices. For use later on, we list the packing fractions: for **bcc**, the pf = .680; for **fcc**, the pf = .740.

## 9. Why are there different lattice types in nature?

For most single atom crystals, such as metals, the normal lattice structure is fcc (or hcp) because it has the highest packing fraction. However, for diatomic molecules, such as NaCl, we can have only one type of atom at a lattice point. The second atom must fit in a hole. For an ionic bonding molecule, it is better energy-wise if the positive ions touch the negative ions but do not touch the other positive ions. Thus, if we locate the bigger of the two atoms at the lattice points, we would **want the smaller atom to be a little bit bigger than the lattice hole size** so it will push the lattice atoms apart, but not too big to leave more empty space. It is a homework assignment (*Problem 6*) to determine which type of lattice NaCl and CsCl would take, given that the Cl ion has a radius of 1.81 Angstroms; the Na ion has a radius of 0.97 Angstroms, and the Cs ion has a radius of 1.67 Angstrom. [An Angstrom = 0.1 nm =  $1 \times 10^{-10}$  m. As you can see, it is a convenient size for atoms.]

## 10. Specifying Planes in a 3-D Lattice and Miller Indices

It is often useful to specify certain planes in a 3-D lattice. The straightforward way is to simply specify three points that lie in the plane but are not colinear. For a lattice, we could simply specify the locations of three lattice points in those planes (that is, **specify an integer to go along with each primitive lattice vector**).

There is another way, much **more convoluted** but it turns out more useful in later work. The procedure is as follows:

1. Find three lattice points in the plane (make sure the plane you choose doesn't go through the origin), i.e., determine the coefficients of  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , and  $\mathbf{a}_3$ . For example, say the points are  $(m\mathbf{a}_1)$ ,  $(n\mathbf{a}_2)$ , and  $(p\mathbf{a}_3)$  where  $m$ ,  $n$ , and  $p$  are integers.
2. Take the reciprocals of these three integers (e.g.,  $1/m$ ,  $1/n$ , and  $1/p$ ).
3. Reduce these three numbers (fractions) to a common denominator (e.g.,  $1/m = np/mnp$ ,  $1/n = mp/mnp$ , and  $1/p = mn/mnp$ ).
4. Simplify if possible (get lowest common denominator).

The resulting numerator values enclosed in parenthesis (**hkl**) is called the index of the plane (see example on the next page). These are sometimes called **Miller Indices**. Note that if the plane does NOT cross a certain direction, then it intersects at infinity and the inverse of infinity is zero.

### Examples:

A plane that runs parallel to the  $yz$  plane (never cuts either the  $y$  or  $z$  plane) and cuts the  $x$  axis at  $1*\mathbf{a}_1$  would be the **(100)** plane – indices would be  $1/1$ ,  $1/\infty$ ,  $1/\infty$  where the symbol  $\infty$  stand for infinity.

A plane that goes through the points  $2\mathbf{a}_1$  and  $3\mathbf{a}_2$  and never crosses  $\mathbf{a}_3$  would have:

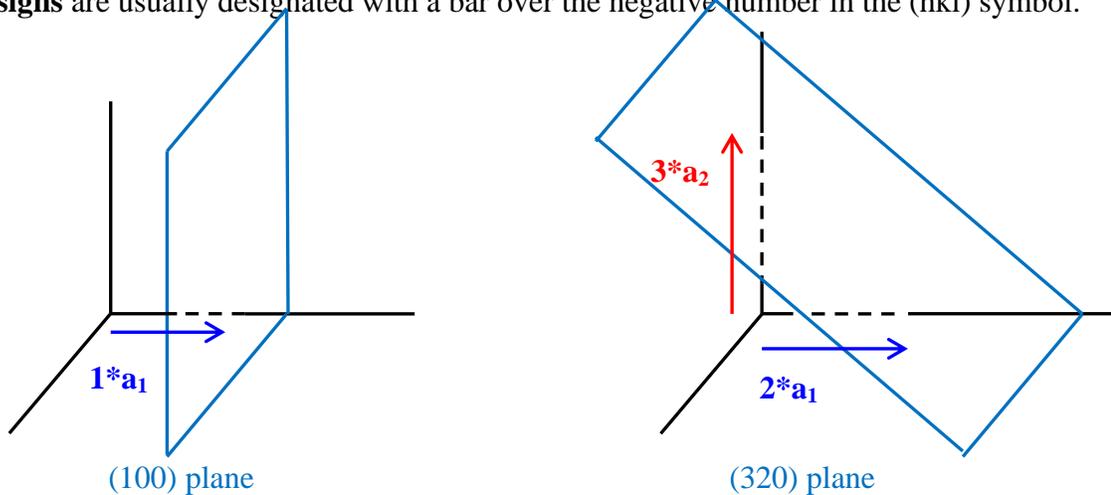
step 1:  $(2, 3, \infty)$

step 2:  $(1/2, 1/3, 0)$

step 3:  $(3/6, 2/6, 0/6)$

step 4:  $(3, 2, 0)$  so the plane would be the **(320)** plane.

**Negative signs** are usually designated with a bar over the negative number in the (hkl) symbol.

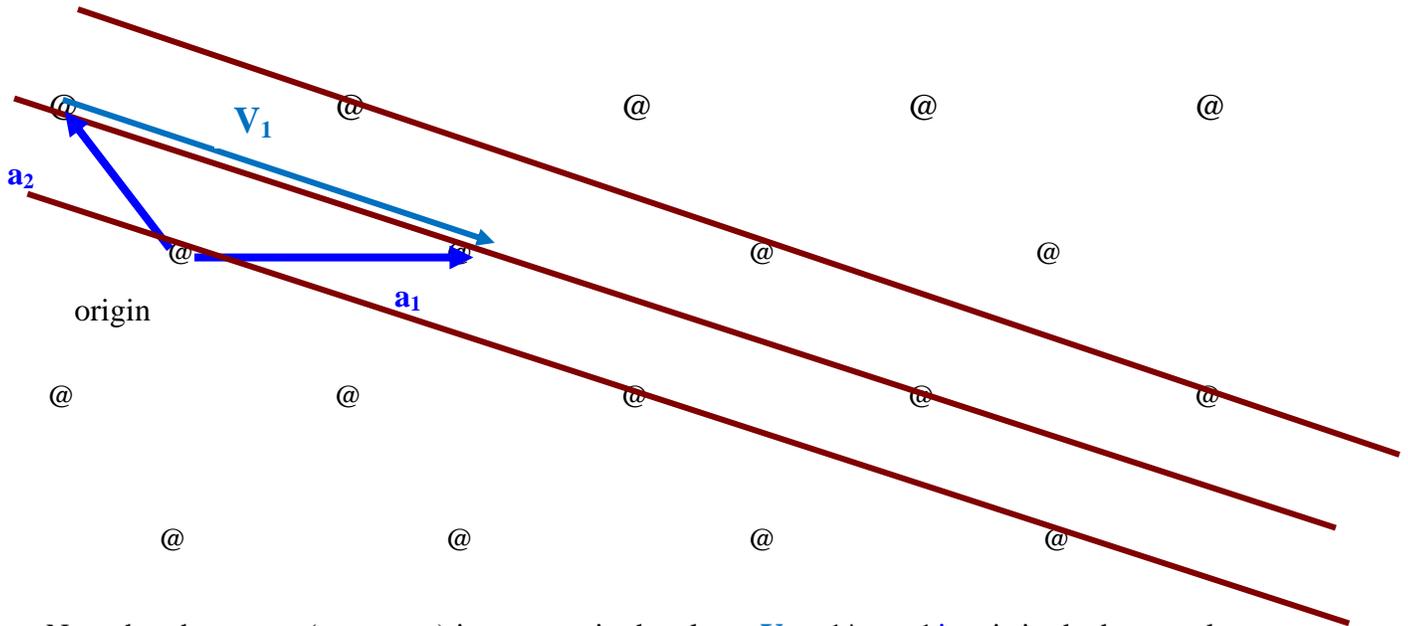


Be careful: the (320) plane comes from  $2\mathbf{a}_1$ ,  $3\mathbf{a}_2$ ,  $\infty\mathbf{a}_3$ , not  $3\mathbf{a}_1$ ,  $2\mathbf{a}_2$ ,  $0\mathbf{a}_3$ .

To draw a **line perpendicular to this plane**, note that the cross product of two vectors in the plane will give a vector perpendicular to each line, and hence perpendicular to the plane. A line in the plane that has points  $(m\mathbf{a}_1)$ ,  $(n\mathbf{a}_2)$ , and  $(p\mathbf{a}_3)$  can be found simply by going from one point to another. The vector  $(m\mathbf{a}_1 - n\mathbf{a}_2)$  is a vector in the plane, and the vector  $(n\mathbf{a}_2 - p\mathbf{a}_3)$  is also in the plane. To find a vector perpendicular to the plane, simply take the cross product of these two vectors.

**Alternate primitive translation vectors:** On the diagram below we show at the top a set of planes and their specification using one set of primitive lattice vectors and the Miller indices that go with that plane, and then below that we show the same set of planes with a different set of primitive lattice vectors and the Miller indices that go with that plane.

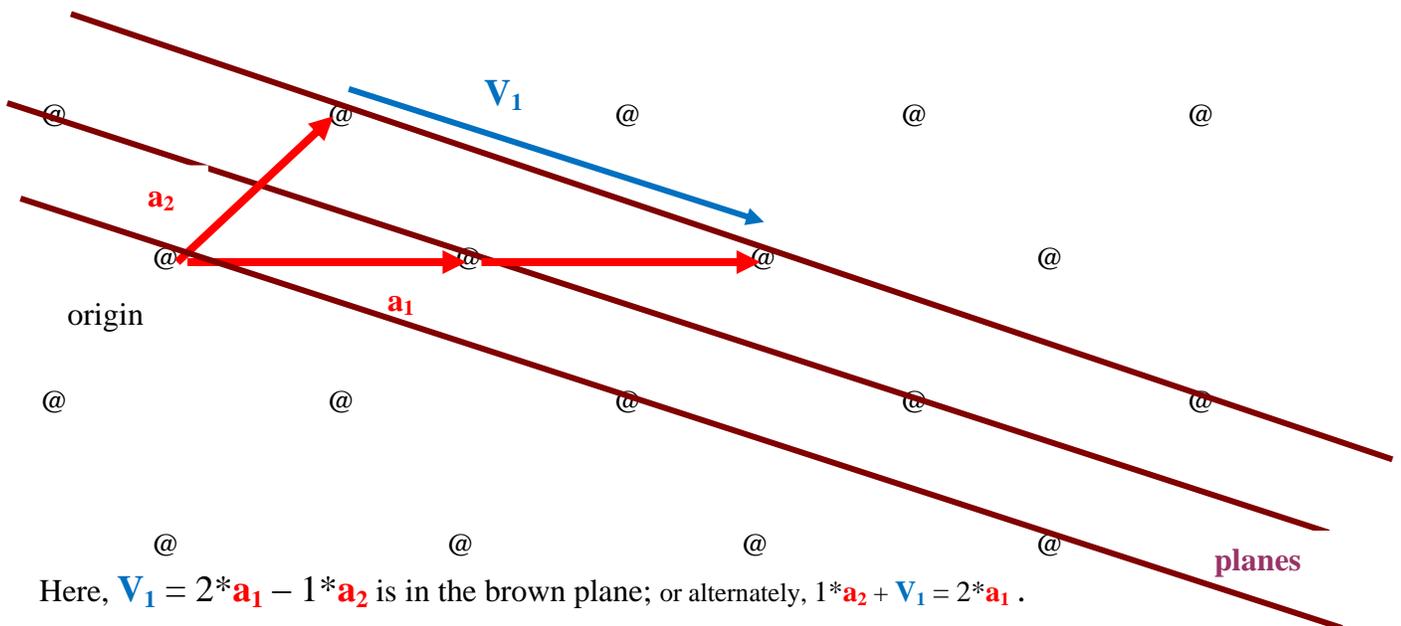
Below we specified the brown plane in terms of the blue primitive translation vectors,  $\mathbf{a}_1$  and  $\mathbf{a}_2$ . Magnified view of the lattice, with the brown planes being  $m=1$ ,  $n=1$ , and  $p$  not specified (since this is just a 2-D intersection of the 3-D plane). If  $p$  is infinity, the Miller Indices would be  $(1,1,0)$ .



Note that the vector  $(m\mathbf{a}_1 - n\mathbf{a}_2)$  is a vector in the plane:  $\mathbf{V}_1 = 1*\mathbf{a}_1 - 1*\mathbf{a}_2$  is in the brown plane.

An alternative way to see this is:  $1\mathbf{a}_2 + \mathbf{V}_1 = 1*\mathbf{a}_1$ .

If we instead use the red primitive translation vectors,  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , the brown plane is specified with  $m=2$ ,  $n=1$ , and  $p$  not specified. If  $p$  is infinite, the Miller Indices would be  $(1,2,0)$ .



Here,  $\mathbf{V}_1 = 2*\mathbf{a}_1 - 1*\mathbf{a}_2$  is in the brown plane; or alternately,  $1*\mathbf{a}_2 + \mathbf{V}_1 = 2*\mathbf{a}_1$ .