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### Lattice Positions and Directions:

- 1) Always establish an origin
- 2) Determine the coordinates of the lattice
- points of interest
- 3) Translate the vector to the origin if
- required by drawing a parallel line or move the origin.
- 4) Subtract the second point from the first: u2-u1,v2-v1,w2-w1
- 5) Clear fractions and reduce to lowest terms
- 6) Write direction with square brackets [uvw]
- 7) Negative directions get a hat.

### **Remember Terminology:**

- •Defined coordinate system: x, y, z
- •Respective unit cell edge lengths: a, b, c
- •Direction: Denoted by [uvw]
- •Family of direction(s): Denoted by: <uvw>
- •Plane: Denoted by: (hkl)
- •Family of Plane(s): Denoted by: {hkl}

•Directions are always perpendicular to their respective planes, i.e. [111] perpendicular (111) (for cubic systems)

•Families of equivalent planes are equal with respect to symmetrical structures, they do not have to be parallel. Equivalent planes must be translated to the correct atomic positions in order to maintain the proper crystal symmetry.

- Families of directions are equivalent in absolute magnitude.
- (222) planes are parallel to the (111) planes but not equal.
- Intercepts for the (222) planes are 1/2, 1/2, 1/2

• Intercepts for the (333) planes are 1/3, 1/3, 1/3, remember this is in what we call "reciprocal space". If you draw out the (333) plane it is parallel to the (111) plane but not equivalent.







# **Density Computations**

Since the entire crystal can be generated by the repetition of the unit cell, the density of a crystalline material,  $\rho$  = the density of the unit cell = (atoms in the unit cell, n)

 $\times$  (mass of an atom, M) / (the volume of the cell, Vc)

Atoms in the unit cell, n = 2 (BCC); 4 (FCC); 6 (HCP)

Mass of an atom, M = Atomic weight, A, in amu (or g/mol) is given in the periodic table. To translate mass from amu to grams we have to divide the atomic weight in amu by the Avogadro number NA =  $6.023 \times 10^{23}$  atoms/mol

The volume of the cell, Vc = a3 (FCC and BCC) a =  $2R\sqrt{2}$  (FCC); a =  $4R/\sqrt{3}$  (BCC) where R is the atomic radius.

### Polycrystalline Materials

• In polycrystalline materials, grain orientations are random, so bulk material properties are isotropic.

• Some polycrystalline materials have grains with preferred orientations (texture), so properties are dominated by those relevant to the texture orientation.

# Polymorphism and Allotropy

Some materials may exist in more than one crystal structure, this is called **polymorphism**. If the material is an elemental solid, it is called allotropy.

An example of allotropy is carbon, which can exist as diamond, graphite, and amorphous carbon.

