**HW#2 Answer Key MSEG 302 Spring 2018**

**a) If the atomic radius of tungsten is 0.137 nm, calculate the volume of its unit cell in cubic nanometers, and the density in g/cm^33.**

The crystal structure of tungsten is BCC, as discussed in the text and lecture. In BCC crystals, the atoms touch along the body diagonal. This means that 4r = Sqrt[3] a, where r is the radius of the atom, and a is the size of the BCC unit cell. For BCC crystals, there are 2 atoms per unit cell. The density is the mass of tungsten atoms in a unit cell, divided the volume of the unit cell itself (a^3 for cubes). So:

a = 4 r / Sqrt[3] = 4 (0.137 nm)/Sqrt [3] =

density = 2 (183.84 amu / Nav) / a3

density = 2 (183.84 g/mol) / (6.02 x 1023 / mol) / a3

To get the units in g/cm3, it is necessary to convert nm to cm.

(\*Mathematica solution\*)

r = 0.137 nm. (\*given in statement\*)

a = 4 r /Sqrt[3] (\*solve for a in terms of r\*)

acm = a (10^-7 cm/ nm) (\*convert a from nm to cm\*)

nav = 6.02 10^23/mol (\*define Avogadro’s number \*)

density = 2 (183.84 g/mol)/nav/acm^3 (\*solve for density\*)

The solution is 19.28 g/cm3, which is close to the value of 19.25 g/cm3 on Wikipedia

**b) Calculate the number of atoms per cubic nanometer in gold.**

The density of gold is 19.32 g/cm^3 (per the table in Callister text). The atomic weight of gold is 196.97 amu (g/mole). So the mass of 1 nm^3 of gold is:

m = (1 nm^3)(10^-7 cm/nm)^3 (19.32 g/cm^3) = 1.932 10^-20 g

The mass of a single gold atom (m1) is 196.97 (g/mole) / Nav = 3.27 10^-22 g/atom.

So the number of atoms in the cubic nanometer is m/m1 = 1.932 10^-20 / 3.27 10^-22 = 59.

Since there are 4 atoms / unit cell (gold is FCC), this corresponds to just under 15 unit cells altogether.

**c) With respect to a cubic unit cell, sketch the following directions:**

**(1) [1 -1 0], (2) [0 0 1], (3) [0 1 -2], (4) [1 2 1], (5) [2 4 2], (6) [-1 2 2], (7) [1 -2 3]**



You can draw this figure however you want (including with a ruler, paper, and pencil), I used Mathematica. Here is the exact code I used if you want to reproduce it:

Graphics3D[{{Opacity[0.05], Cuboid[{0, 0, 0}, {1, 1, 1}]},

{Text["[1 -1 0]", {1, -1, 0}], Arrow[{{0, 0, 0}, {1, -1, 0}}]},

{Text["[0 0 1]", {0, 0, 1}], Arrow[{{0, 0, 0}, {0, 0, 1}}]},

{Text["[0 1 -2]", {0, 1, -2}], Arrow[{{0, 0, 0}, {0, 1, -2}}]},

{Text["[1 2 1]", {1, 2, 1}], Arrow[{{0, 0, 0}, {1, 2, 1}}]},

{Text["[2 4 2]", {2, 4, 2}], Arrow[{{0, 0, 0}, {2, 4, 2}}]},

{Text["[-1 2 2]", {-1, 2, 2}], Arrow[{{0, 0, 0}, {-1, 2, 2}}]},

{Text["[1 -2 3]", {1, -2, 3}], Arrow[{{0, 0, 0}, {1, -2, 3}}]},

{Red, Arrow[{{0, 0, 0}, {1, 0, 0}}]}, {Green,

Arrow[{{0, 0, 0}, {0, 1, 0}}]}, {Blue,

Arrow[{{0, 0, 0}, {0, 0, 1}}]}}, Axes -> True,

AxesLabel -> {"x", "y", "z"}]

**d) With respect to a cubic unit cell, sketch the following planes:**

**(1) (1 -1 0), (2) (0 0 1), (3) (0 1 -2), (4) (1 2 1), (5) (2 4 2), (6) (-1 2 2), (7) (1 -2 3)**



Again, here is the detailed Mathematica code for making the plot. I used “opacity” to make the planes a bit transparent. For planes that are parallel to one or more of the axes I used polygon, and for the others I used triangle. Also, as was pointed out in class, my initial drawing shown in class for the (0 1 -2) plane was incorrect; the corrected version is shown here. Let me know if you find any other errors.

Graphics3D[{{Opacity[0.05], Cuboid[{0, 0, 0}, {1, 1, 1}]},

{Opacity[0.5], Polygon[{{1, 0, 0}, {0, -1, 0}, {0, -1, 1}, {1, 0, 1}}]},

{Opacity[0.5], Polygon[{{1, 0, 1}, {1, 1, 1}, {0, 1, 1}, {0, 0, 1}}]},

{Opacity[0.5], Polygon[{{0, 1, 0}, {0, 0, -1/2}, {1, 0, -1/2}, {1, 1, 0}}]},

{Opacity[0.5], Triangle[{{1/1, 0, 0}, {0, 1/2, 0}, {0, 0, 1/1}}]},

{Opacity[0.5], Triangle[{{1/2, 0, 0}, {0, 1/4, 0}, {0, 0, 1/2}}]},

{Opacity[0.5], Triangle[{{1/-1, 0, 0}, {0, 1/2, 0}, {0, 0, 1/2}}]},

{Opacity[0.5], Triangle[{{1, 0, 0}, {0, -1/2, 0}, {0, 0, 1/3}}]},

{Red, Arrow[{{0, 0, 0}, {1, 0, 0}}]}, {Green,

Arrow[{{0, 0, 0}, {0, 1, 0}}]}, {Blue,

Arrow[{{0, 0, 0}, {0, 0, 1}}]}}, Axes -> True,

AxesLabel -> {"x", "y", "z"}]

**e) Calculate the radius of a palladium (Pd) atom, given that the crystal structure is FCC, the density is 12.0 g/cm3, and the atomic weight is 106.4 g/mol.**

For FCC, the atoms touch along the face diagonal, so Sqrt[2] a = 4 r (eqn 1). There are 4 atoms in the unit cell, so the density = 4 (106.4 g/mol) / Nav / a^3 (eqn 2). Given that density = 12.0 g/cm3 (again using Nav = 6.02 10^23 / mol and 1 cm = 10^ -7 nm), solving equation (2) for a, and then (1) for r gives r = 0.137 nm.

**f) Iron undergoes an allotropic transformation from BCC (alpha, ferrite) to FCC (gamma, austenite) upon heating to a temperature of 912 C. At this transition, the atomic radius abruptly changes from RBCC = 0.126 nm to RFCC = 0.129 nm. From this information, calculate the expected density of BCC iron, as well as the expected density of FCC iron.**

For BCC iron, atoms meet along body diagonal, so Sqrt[3] a = 4 r. Since rbcc = 0.126, this gives aBCC =

For FCC iron, atoms meet along face diagonal, so Sqrt[2] a = 4 r.

The atomic weight of iron is 55.845 amu = 55.845 g/mol. So density for BCC iron = 2 (55.845 g/mol)/Nav / aBCC^3 = 7.53 g/cm^3.

For FCC iron, 4 (55.845)/Nav/.aFCC^3 = 7.64 g/cm^3.

Note that FCC iron is denser than BCC iron, but also has the bigger crystal vacancy in the structure. Again, this is why hot iron is ductile (FCC metals deform more easily), and will dissolve more carbon (~2 wt% vs. only 0.02 wt% in BCC iron).