Body-centered cubic problems

Problem #1: The edge length of the unit cell of Ta, is 330.6 pm; the unit cell is body-centered cubic. Tantalum has a density of 16.69 g/cm^3.

(a) calculate the mass of a tantalum atom.
(b) Calculate the atomic weight of tantalum in g/mol.

Solution:

1) Convert pm to cm:

330.6 pm x 1 cm/10^{10} pm = 330.6 x 10^{-10} cm = 3.306 x 10^{-8} cm

2) Calculate the volume of the unit cell:

(3.306 x 10^{-8} cm)^3 = 3.6133 x 10^{-23} cm^3

3) Calculate mass of the 2 tantalum atoms in the body-centered cubic unit cell:

16.69 g/cm^3 times 3.6133 x 10^{-23} cm^3 = 6.0307 x 10^{-22} g

4) The mass of one atom of Ta:

6.0307 x 10^{-22} g / 2 = 3.015 x 10^{-22} g

5) The atomic weight of Ta in g/mol:

3.015 x 10^{-22} g times 6.022 x 10^{23} mol^{-1} = 181.6 g/mol

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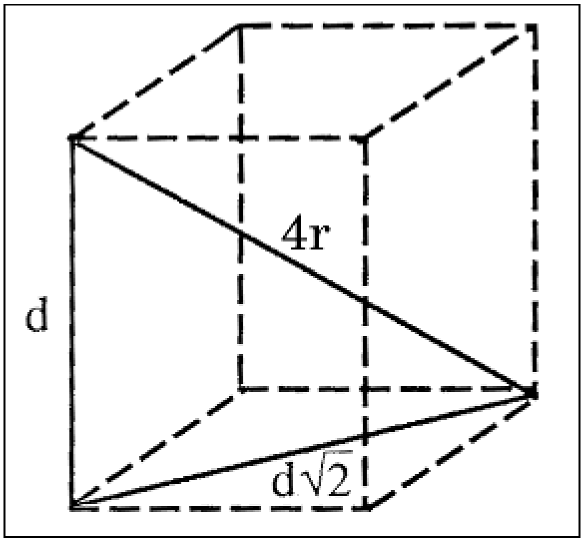
Problem #2a: Chromium crystallizes in a body-centered cubic structure. The unit cell volume is 2.583 x 10^{-23} cm^3. Determine the atomic radius of Cr in pm.

Solution:

1) Determine the edge length of the unit cell:

2.583 x 10^{-23} cm^{3}3 = 2.956 x 10^{-8} cm

2) Examine the following diagram:



The triangle we will use runs differently than the triangle used in fcc calculations.
d is the edge of the unit cell, however d√2 is NOT an edge of the unit cell. It is a diagonal of a face of the unit cell. 4r is a body diagonal. Since it is a right triangle, the Pythagorean Theorem works just fine.

We wish to determine the value of 4r, from which we will obtain r, the radius of the Cr atom. Using the Pythagorean Theorem, we find:

$d^2 + (d2)^2 = (4r)^2$

$3d^2 = (4r)^2$

$3(2.956 \times 10^{-8}\text{ cm})^2 = 16r^2$

$r = 1.28 \times 10^{-8}$ cm

3) The conversion from cm to pm is left to the student.

Problem #2b: Chromium crystallizes with a body-centered cubic unit cell. The radius of a chromium atom is 128 pm . Calculate the density of solid crystalline chromium in grams per cubic centimeter.

Solution:

1) Convert pm to cm:

$(125\text{ pm})\ (1\text{ cm} / 10^{10}\text{ pm}) = 1.25 \times 10^{-8}$ cm

2) Use the Pythagorean theorem to calculate the unit cell edge length:

$d^2 + (d2)^2 = (4r)^2$

$3d^2 = (4r)^2$

$3d^2 = 16r^2$

$3d^2 = (16) (1.25 \times 10^{-8}\text{ cm})^2$

$d3 = (4) (1.25 \times 10^{-8}\text{ cm})$

$d = [(4) (1.25 \times 10^{-8}\text{ cm})] / 3$

$d = 2.8868 \times 10^{-8}$ cm

3) Calculate volume of the unit cell

$(2.8868 \times 10^{-8}\text{ cm})^3 = 2.4056 \times 10^{-23}\text{ cm}^3$

4) Determine mass of two atoms in body-centered unit cell:

51.996 g/mol / 6.022×10^{23} atoms/mol = 8.63434×10^{-23} g/atom

8.63434×10^{-23} g/atom times 2 = 1.726868×10^{-22} g

5) Determine the density:

$1.726868 \times 10^{-22}\text{ g} / 2.4056 \times 10^{-23}\text{ cm}^3 = 7.18\text{ g/cm}^3$ (to three sig figs)

Book value is 7.15.

Problem #3: Barium has a radius of 224 pm and crystallizes in a body-centered cubic structure. What is the edge length of the unit cell? (This is the reverse of problem #4.)

Solution:

1) Calculate the value for 4r (refer to the above diagram):

radius for barium = 224 pm

4r = 896 pm

2) Apply the Pythagorean Theorem:

$d^2 + (d2)^2 = (896)^2$

$3d^2 = 802816$

$d^2 = 267605.3333. . .$

d = 517 pm

Problem #4: Metallic potassium has a body-centered cubic structure. If the edge length of unit cell is 533 pm, calculate the radius of potassium atom. (This is the reverse of problem #3.)

Solution:

1) Solve the Pythagorean Theorem for r (with d = the edge length):

$d^2 + (d2)^2 = (4r)^2$

$d^2 + 2d^2 = 16r^2$

$3d^2 = 16r^2$

$r^2 = 3d^2 / 16$

r = (d3) / 4

2) Solve the problem:

r = (5333) / 4

r = 231 pm

Problem #5: Sodium has a density of 0.971 g/cm^3 and crystallizes with a body-centered cubic unit cell. (a) What is the radius of a sodium atom? (b) What is the edge length of the cell? Give answers in picometers.

Solution:

1) Determine mass of two atoms in a bcc cell:

22.99 g/mol divided by 6.022×10^{23} mol^{-1} = 3.81767×10^{-23} g (this is the average mass of one atom of Na)

3.81767×10^{-23} g times 2 = 7.63534×10^{-23} g

2) Determine the volume of the unit cell:

7.63534×10^{-23} g divided by 0.971 g/cm^3 = 7.863378×10^{-23} cm^3

3) Determine the edge length, which is the answer to (b):

7.863378×10^{-23} $cm^3 3$ = 4.2842×10^{-8} cm

4) Use the Pythagorean Theorem (refer to above diagram):

$d^2 + (d2)^2 = (4r)^2$

$3d^2 = 16r^2$

$r^2 = 3(4.2842 \times 10^{-8})^2 / 16$

$r = 1.855 \times 10^{-8}$ cm

5) The radius of the sodium atom is 185.5 pm. The edge length is 428.4 pm. The manner of these conversions are left to the reader.

Problem #6: At a certain temperature and pressure an element has a simple body-centred cubic unit cell. The corresponding density is 4.253 g/cm^3 and the atomic radius is 1.780 Å. Calculate the atomic mass (in amu) for this element.

Solution:

1) Convert 1.780 Å to cm:

1.780 Å = 1.780×10^{-8} cm

2) Use the Pythagorean Theorem to calculate d, the edge length of the unit cell:

$d^2 + (d2)^2 = (4r)^2$

$3d^2 = 16r^2$

$d^2 = (16/3)\ (1.780 \times 10^{-8}\ cm)^2$

$d = 4.11 \times 10^{-8}$ cm

3) Calcuate the volume of the unit cell:

$(4.11 \times 10^{-8}\ cm)^3 = 6.95 \times 10^{-23}\ cm^3$

4) Calcuate the mass inside the unit cell:

$6.95 \times 10^{-23}\ cm^3$ times $4.253\ g/cm^3 = 2.95 \times 10^{-22}$ g

5) Use a ratio and proportion to calculate the atomic mass:

2.95×10^{-22} g is to two atoms as 'x' is to $6.022 \times 10^{23}\ mol^{-1}$

x = 88.95 g/mol (or 88.95 amu)

Problem #7: Mo crystallizes in a body-centered cubic arrangement. Calculate the radius of one atom, given the density of Mo is 10.28 g /cm^3.

Solution:

1) Determine mass of two atoms in a bcc cell:

95.96 g/mol divided by $6.022 \times 10^{23}\ mol^{-1} = 1.59349 \times 10^{-22}$ g (this is the average mass of one atom of Mo)

1.59349×10^{-22} g times 2 = 3.18698×10^{-22} g

2) Determine the volume of the unit cell:

3.18698×10^{-22} g divided by $10.28\ g/cm^3 = 3.100175 \times 10^{-23}\ cm^3$

3) Determine the edge length:

$3.100175 \times 10^{-23}\ cm^33 = 3.14144 \times 10^{-8}$ cm

4) Use the Pythagorean Theorem (refer to above diagram):

$d^2 + (d2)^2 = (4r)^2$

$3d^2 = 16r^2$

$r^2 = 3(3.14144 \times 10^{-8})^2 / 16$

$r = 1.3603 \times 10^{-8}$ cm (or 136.0 pm, to four sig figs)

Problem #8: Sodium crystallizes in body-centered cubic system, and the edge of the unit cell is 430. pm. Calculate the dimensions of a cube that would contain one mole of Na.

Solution:

A cube that is bcc has two atoms per unit cell.

6.022×10^{23} atoms divided by 2 atoms/cell = 3.011×10^{23} cells required.

430. pm = 4.30×10^{-8} cm <--- I'm going to give the answer in cm^3 rather than pm^3

$(4.30 \times 10^{-8}\ cm)^3 = 7.95 \times 10^{-23}\ cm^3$ <--- vol. of unit cell in cm^3

$(3.011 \times 10^{23}\ cell)\ (7.95 \times 10^{-23}\ cm^3/cell) = 23.9\ cm^3$

23.9 cm^3 would be a cube 2.88 cm on a side (2.88 being the cube root of 23.9)

Problem #9: Vanadium crystallizes with a body-centered unit cell. The radius of a vanadium atom is 131 pm. Calculate the density of vanadium in g/cm^3.

Solution:

1) We are going to use the Pythagorean Theorem to determine the edge length of the unit cell. That edge length will give us the volume.

131 pm times (1 cm / 10^{10} pm) = 131×10^{-10} cm = 1.31×10^{-8} cm

The right triangle for Pythagorean Theorem is here. The image is in problem #2.

$3d^2 = (4 * 1.31 \times 10^{-8}\ cm)^2$

$d^2 = (4 * 1.31 \times 10^{-8}\ cm)^2 / 3$

d = 3.0253×10^{-8} cm <--- this is the edge length

Cube the edge length to give the volume:

2.7689×10^{-23} cm^3

2) We will use the average mass of one V atom and the two atoms in bcc to determine the mass of V inside the unit cell.

50.9415 g/mol divided by 6.022×10^{23} mol^{-1} = 8.459×10^{-23} g <--- average mass of one atom

8.459×10^{-23} g times 2 = 1.6918×10^{-22} g <--- mass of V in unit cell

3) Step 2 divided by step 1 gives the density.

1.6918×10^{-22} g / 2.7689×10^{-23} cm^3 = 6.11 g/cm^3

Problem #10: Titanium metal has a body-centered cubic unit cell. The density of titanium is 4.50 g/cm^3. Calculate the edge length of the unit cell and a value for the atomic radius of titanium. (Hint: In a body-centered arrangement of spheres, the spheres touch across the body diagonal.)

Solution:

1) We need to determine the volume of one unit cell. I'll approach this in a dimensional analysis sorta way:

(volume/g) (g/mole) (mole/atoms) (atoms/cell) = (volume/cell)

See how all the units cancel except for volume and cell. Once we have the volume of the cell, we can determine the edge lenth by taking the cube root of the volume.

I'll build it one calculation at a time.

2) (volume/g)

1.00 cm^3/4.50 g

3) (volume/g) (g/mole) <--- molar mass of Ti

(1.00 cm^3/4.50 g) (47.867 g/mol)

4) (volume/g) (g/mole) (mole/atoms) <--- Avogadro's Number

(1.00 cm^3/4.50 g) (47.867 g/mol) (1.00 mol/6.022 x 10^{23} atoms)

5) (volume/g) (g/mole) (mole/atoms) (atoms/cell)

(1.00 cm^3/4.50 g) (47.867 g/mol) (1.00 mol/6.022 x 10^{23} atoms) (2 atoms/cell) <--- because of body-centered cubic

6) Do the calculation for the volume of the unit cell. The answer is:

3.53275 x 10^{-23} cm^3

7) The edge length is simply the cube root of the cell volume. The answer is:

3.28 x 10^{-8} cm (to three sig figs)

Comment: often the edge length is asked for in pm. The student is left to determine the conversion from cm to pm. The answer is 328 pm.

8) For the atomic radius, I will add some guard digits to the edge length (symbolized by 'd' in the Pythagorean theorem calculation I will use. By the way, remember that hint from the problem text? That's the thing that allows me to write 4r.

$d^2 + (d2)^2 = (4r)^2$

$(4r)^2 = 3d^2$

$16r^2 = 3d^2$

$r^2 = 3d^2 / 16$

$r = d3 / 4$

r = [(3.28124 x 10^{-8} cm) (3)] / 4

r = 1.42 x 10^{-8} cm = 142 pm

Bonus Problem: In modeling solid-state structures, atoms and ions are most often modeled as spheres. A structure built using spheres will have some empty space in it. A measure of the empty (also called void) space in a particular structure is the packing efficiency, defined as the volume occupied by the spheres divided by the total volume of the structure.

Given that a solid crystallizes in a body-centered cubic structure that is 3.05 Å on each side, please answer the following questions.

Solution:

a. How many atoms are there in each unit cell?

2

b. What is the volume of one unit cell in $Å^3$?

$(3.05\ Å)^3 = 28.372625\ Å^3$

c. Assuming that the atoms are spheres and the radius of each sphere is 1.32 Å, what is the volume of one atom in $Å^3$?

$(4/3)\ (3.141592654)\ (1.32)^3 = 9.63343408\ Å^3$

I used the key for π on my calculator, so there were some internal digits in addition to that last 4 (which is actually rounded up from the internal digits).

d. Therefore, what volume of atoms are in one unit cell?

$(9.63343408\ Å^3 \text{ times } 2) = 19.26816686\ Å^3$

e. Based on your results from parts b and d, what is the packing efficiency of the solid expressed as a percentage?

$19.26816686\ Å^3 / 28.372625\ Å^3 = 0.679$

67.9%

Face-centered cubic problems

Problem #1: Palladium crystallizes in a face-centered cubic unit cell. Its density is 12.023 g/cm^3. Calculate the atomic radius of palladium.

Solution:

1) Calculate the average mass of one atom of Pd:

106.42 g mol^{-1} ÷ 6.022 x 10^{23} atoms mol^{-1} = 1.767187 x 10^{-22} g/atom

2) Calculate the mass of the 4 palladium atoms in the face-centered cubic unit cell:

1.767187 x 10^{-22} g/atom times 4 atoms/unit cell = 7.068748 x 10^{-22} g/unit cell

3) Use density to get the volume of the unit cell:

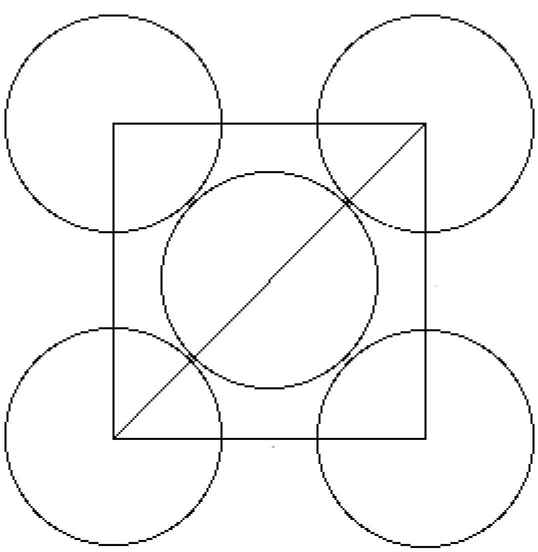
7.068748 x 10^{-22} g ÷ 12.023 g/cm^3 = 5.8793545 x 10^{-23} cm^3

4) Determine the edge length of the unit cell:

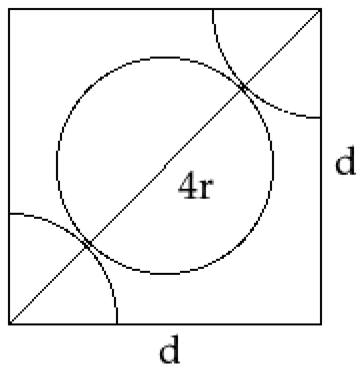
5.8793545 x 10^{-23} cm^{3}3 = 3.88845 x 10^{-8} cm

5) Determine the atomic radius:

Remember that a face-centered unit cell has an atom in the middle of each face of the cube. The square represents one face of a face-centered cube:



Here is the same view, with 'd' representing the side of the cube and '4r' representing the 4 atomic radii across the face diagonal.



Using the Pythagorean Theorem, we find:

$d^2 + d^2 = (4r)^2$

$2d^2 = 16r^2$

$r^2 = d^2 \div 8$

$r = d \div \sqrt{8}$ <--- often left like this

$r = d \div 2(\sqrt{2})$ <--- an alternate formulation

$r = 1.3748 \times 10^{-8}$ cm

You may wish to convert the cm value to picometers, the most common measurement used in reporting atomic radii. Try it before looking at the solution to the next problem.

The above discusses how to determine r in terms of d in a face-centered unit cell. You may be asked to do the opposite, that is, to determine d in terms of r for a fcc cell. I'll repeat:

$r = d \div \sqrt{8}$

followed by a simple rearrangement:

$d = r\sqrt{8}$

Problem #2: Nickel crystallizes in a face-centered cubic lattice. If the density of the metal is 8.908 g/cm^3, what is the unit cell edge length in pm?

Solution:

This problem is like the one above, it just stops short of determining the atomic radius.

1) Calculate the average mass of one atom of Ni:

58.6934 g mol^{-1} ÷ 6.022 x 10^{23} atoms mol^{-1} = 9.746496 x 10^{-23} g/atom

2) Calculate the mass of the 4 nickel atoms in the face-centered cubic unit cell:

9.746496 x 10^{-23} g/atom times 4 atoms/unit cell = 3.898598 x 10^{-22} g/unit cell

3) Use density to get the volume of the unit cell:

3.898598 x 10^{-22} g ÷ 8.908 g/cm^3 = 4.376514 x 10^{-23} cm^3

4) Determine the edge length of the unit cell:

4.376514 x 10^{-23} cm^{3}3 = 3.524 x 10^{-8} cm

5) Convert cm to pm:

cm = 10^{-2} m; pm = 10^{-12} m.

Consequently, there are 10^{10} pm/cm

(3.524 x 10^{-8} cm) (10^{10} pm/cm) = 352.4 pm

Problem #3: Nickel has a face-centered cubic structure with an edge length of 352.4 picometers. What is the density?

This problem is the exact reverse of problem #2. (See problem 5a below for an example set of calculations.)

Solution:

1) Convert pm to cm
2) Calculate the volume of the unit cell
3) Calculate the average mass of one atom of Ni
4) Calculate the mass of the 4 nickel atoms in the face-centered cubic unit cell
5) Calculate the density (value from step 4 divided by value from step 2)

Problem #4: Calcium has a cubic closest packed structure as a solid. Assuming that calcium has an atomic radius of 197 pm, calculate the density of solid calcium.

Solution:

1) Convert pm to cm:

197 pm x (1 cm/10^{10} pm) = 1.97 x 10^{-8} cm

2) Determine the edge length of the unit cell:

Use the Pythagorean Theorem (see problem #1 for a discussion):

r = d ÷ 2(√2) <--- one of two alternate formulations

1.97 x 10^{-8} cm = d ÷ 2(√2)

d = 5.572 x 10^{-8} cm

3) Determine the volume of the unit cell:

(5.572 x 10^{-8} cm$)^3$ = 1.730 x 10^{-22} cm^3

4) Determine mass of 4 atoms of Ca in a unit cell (cubic closest packed is the same as face-centered cubic):

40.08 g/mol divided by 6.022 x 10^{23} atoms/mol = 6.6556 x 10^{-23} g/atom

6.6556 x 10^{-23} g/atom times 4 atoms = 2.66224 x 10^{-22} g

5) Determine density:

2.66224 x 10^{-22} g divided by 1.730 x 10^{-22} cm^3 = 1.54 g/cm^3

Problem #5: Krypton crystallizes with a face-centered cubic unit cell of edge 559 pm.

a) What is the density of solid krypton?
b) What is the atomic radius of krypton?
c) What is the volume of one krypton atom?
d) What percentage of the unit cell is empty space if each atom is treated as a hard sphere?

Solution to a:

1) Convert pm to cm:

559 pm x (1 cm/10^{10} pm) = 559 x 10^{-10} cm = 5.59 x 10^{-8} cm

2) Calculate the volume of the unit cell:

(5.59 x 10^{-8} cm)^3 = 1.7468 x 10^{-22} cm^3

3) Calculate the average mass of one atom of Kr:

83.798 g mol^{-1} divided by 6.022 x 10^{23} atoms mol^{-1} = 1.39153 x 10^{-22} g

4) Calculate the mass of the 4 krypton atoms in the face-centered cubic unit cell:

1.39153 x 10^{-22} g times 4 = 5.566 x 10^{-22} g

5) Calculate the density (value from step 4 divided by value from step 2):

5.566 x 10^{-22} g / 1.7468 x 10^{-22} cm^3 = 3.19 g/cm^3

Solution to b:

Use the Pythagorean Theorem (see problem #1 for a discussion):

r = d ÷ √8 <--- one of two alternate formulations

r = 5.59 x 10^{-8} cm ÷ √8

r = 1.98 x 10^{-8} cm

Solution to c:

$V = (4/3)\ \pi\ r^3$

$V = (4/3)\ (3.14159)\ (1.98 \times 10^{-8}\ \text{cm})^3$

$V = 3.23 \times 10^{-23}\ \text{cm}^3$

Solution to d:

1) Calculate the volume of the 4 atoms in the unit cell:

$3.23 \times 10^{-23}\ \text{cm}^3$ times $4 = 1.29 \times 10^{-22}\ \text{cm}^3$

2) Calculate volume of cell not filled with Kr:

$1.7468 \times 10^{-22}\ \text{cm}^3$ minus $1.29 \times 10^{-22}\ \text{cm}^3 = 4.568 \times 10^{-23}\ \text{cm}^3$

3) Calculate % empty space:

$4.568 \times 10^{-23}\ \text{cm}^3$ divided by $1.7468 \times 10^{-22}\ \text{cm}^3 = 0.2615$

26%

Problem #6: You are given a small bar of an unknown metal. You find the density of the metal to be 11.5 g/cm^3. An X-ray diffraction experiment measures the edge of the face-centered cubic unit cell as 4.06×10^{-10} m. Find the gram-atomic weight of this metal and tentatively identify it.

Solution:

1) Convert meters to cm:

$4.06 \times 10^{-10}\ \text{m} = 4.06 \times 10^{-8}\ \text{cm}$

2) Determine the volume of the unit cube:

$(4.06 \times 10^{-8}\ \text{cm})^3 = 6.69234 \times 10^{-23}\ \text{cm}^3$

3) Determine the mass of the metal in the unit cube:

$11.5\ \text{g/cm}^3$ times $6.69234 \times 10^{-23}\ \text{cm}^3 = 7.696193 \times 10^{-22}\ \text{g}$

4) Determine atomic weight (based on 4 atoms per unit cell):

7.696193×10^{-22} g is to 4 atoms as x grams is to 6.022×10^{23} atoms

x = 116 g/mol (to three sig figs)

This weight is close to that of indium.

Problem #7: A metal crystallizes in a face-centered cubic lattice. The radius of the atom is 0.197 nm. The density of the element is 1.54 g/cm^3. What is this metal?

Solution:

1) Convert nm to cm:

0.197 nm x (1 cm/10^7 nm) = 1.97×10^{-8} cm

2) Determine the edge length of the unit cell:

Use the Pythagorean Theorem (see problem #1 for a discussion):

r = d ÷ 2(√2) <--- one of two alternate formulations

1.97×10^{-8} cm = d ÷ 2(√2)

d = 5.572×10^{-8} cm

3) Determine the volume of the unit cell:

$(5.572 \times 10^{-8}\ \text{cm})^3 = 1.72995 \times 10^{-22}\ \text{cm}^3$

4) Determine grams of metal in unit cell:

1.72995×10^{-22} cm^3 times 1.54 g/cm^3 = 2.6641×10^{-22} g

5) Determine atomic weight (based on 4 atoms per unit cell):

2.6641×10^{-22} g is to 4 atoms as x grams is to 6.022×10^{23} atoms

x = 40.11 g/mol

The metal is calcium.

Problem #8: The density of an unknown metal is 2.64 g/cm^3 and its atomic radius is 0.215 nm. It has a face-centered cubic lattice. Determine its atomic weight.

Solution:

1) Convert nm to cm:

0.215 nm x (1 cm/10^7 nm) = 2.15 x 10^{-8} cm

2) Determine the edge length of the unit cell:

Use the Pythagorean Theorem (see problem #1 for a discussion):

r = d ÷ √8 <--- one of two alternate formulations

2.15 x 10^{-8} cm = d ÷ √8

d = 6.08112 x 10^{-8} cm

3) Determine the volume of the unit cell:

(6.08112 x 10^{-8} cm)^3 = 2.2488 x 10^{-22} cm^3

4) Determine grams of metal in unit cell:

2.2488 x 10^{-22} cm^3 times 2.64 g/cm^3 = 5.9368 x 10^{-22} g

5) Determine atomic weight (based on 4 atoms per unit cell):

5.9368 x 10^{-22} g is to 4 atoms as x grams is to 6.022 x 10^{23} atoms

x = 89.4 g/mol

Problem #9: Metallic silver crystallizes in a face-centered cubic lattice with L as the length of one edge of the unit cube. What is the center-to-center distance between nearest silver atoms?

A) L / 2
B) $2^{½}$ L
C) 2L
D) L / $2^{½}$
E) None of the above answers are valid.

Solution:

Call center-to-center distance = d. There are two of them on the face diagonal.

Therefore, by the Pythagorean Theorem:

$L^2 + L^2 = (2d)^2$

$2L^2 = 4d^2$

$(L^2) / 2 = d^2$

$L / 2^{½} = d$

Answer choice D.

Problem #10: Iridium has a face-centered cubic unit cell with an edge length of 383.3 pm. The density of iridium is 22.61 g/cm^3. Use these data to calculate a value for Avogadro's Number.

Solution:

1) Use the edge length to get the volume of the unit cell:

383.3 pm = 3.833×10^{-8} cm

$(3.833 \times 10^{-8}\ cm)^3 = 5.6314 \times 10^{-23}\ cm^3$

2) Use the density to get the mass of Ir in the unit cell:

22.61 g/cm^3 times $5.6314 \times 10^{-23}\ cm^3 = 1.27326 \times 10^{-21}$ g

3) Use the atomic weight of Ir to determine how many moles of Ir are in the unit cell:

1.27326×10^{-21} g divided by 192.217 g/mol = 6.624075×10^{-24} mol

4) Use 4 atoms per face-centered unit cell to set up the following ratio and proportion:

4 atoms is to 6.624075×10^{-24} mol as x is to 1.000 mol

$x = 6.038 \times 10^{23}$ atoms

For a different take on the solution to this problem, go here and take a look at the answer by Dr W.

Problem #11: Platinum has a density of 21.45 g/cm^3 and a unit cell side length 'd' of 3.93 Ångstroms. What is the atomic radius of platinum? (1 Å = 10^{-8} cm.)

Solution:

1) We need to determine if the unit cell is fcc or bcc.

Volume of unit cell:
$(3.93 \times 10^{-8}\ \text{cm})^3 = 6.0698 \times 10^{-23}\ \text{cm}^3$

Determine the mass of Pt in the unit cell:

21.45 g/cm^3 times 6.0698×10^{-23} cm^3 = 1.302×10^{-21} g

How many atoms is that?

$(1.302 \times 10^{-21}\ \text{g} / 195.078\ \text{g/mol}) * 6.022 \times 10^{23}\ \text{mol}^{-1} = 4$

The unit cell for Pt is fcc.

2) Use the Pythogrean Theorem to calculate the length of the hypotenuse which we know to be four times the radii of one Pt atom (see Problem #1 for a discussion).

We know this:
$d^2 + d^2 = (4r)^2$ <--- where d is the edge length and r is the radius of the atom.

Therefore:

$r = d \div 2(\sqrt{2})$ <--- one of two alternate formulations

$r = (3.93 \times 10^{-8}\ \text{cm}) \div 2(\sqrt{2})$

r = 1.39×10^{-8} cm

3) Note that picometers is the preferred unit for atomic radii (with Ångstroms being the preferred unit of older vintage (for example, when the ChemTeam was in school).

1.39×10^{-8} cm equals:
139 pm
1.39 Å

Problem #12: The unit cell of platinum has a length of 392.0 pm along each side. Use this length (and the fact that Pt has a face-centered unit cell) to calculate the density of platinum metal in kg/m^3 (Hint: you will need the atomic mass of platinum and Avogadro's number).

Solution:

1) Calculate the volume of the unit cell in meters cubed:

392.0 pm times (1 m / 10^{12} pm) = 392.0×10^{-12} m = 3.920×10^{-10} m

$(3.920 \times 10^{-10} \text{ m})^3 = 6.0236288 \times 10^{-29} \text{ m}^3$

2) Calculate the mass of Pt in the unit cell in kg:

195.078 g/mol divided by 6.022×10^{23} mol^{-1} = 3.239422×10^{-22} g

3.239422×10^{-22} g times 4 = $1.2957688 \times 10^{-21}$ g

$1.2957688 \times 10^{-21}$ g times (1 kg / 1000 g) = $1.2957688 \times 10^{-24}$ kg

3) Calculate the density:

$1.2957688 \times 10^{-24}$ kg / $6.0236288 \times 10^{-29}$ m^3 = 21511 kg / m^3

The book value is 21450 kg / m^3.

Note the use of the SI-approved unit for density as opposed to the more commonly-used unit of g/cm^3.

Problem #13: A metal crystallizes in a face-centered cubic structure and has a density of 11.9 g cm^{-3}. If the radius of the metal atom is 138 pm, what is the most probable identity of the metal.

Solution:

1) Determine the atom radius in cm:

138 pm times (100 cm / 10^{12} pm) = 138 x 10^{-10} cm = 1.38 x 10^{-8} cm

2) Determine the edge length of the unit cell:

Use the Pythagorean Theorem (see problem #1 for a discussion):

r = d ÷ √8 <--- one of two alternate formulations

1.38 x 10^{-8} cm = d ÷ √8

d = 3.90323 x 10^{-8} cm

2) Determine the volume of the unit cell:

(3.90323 x 10^{-8} cm$)^3$ = 5.94665 x 10^{-23} cm^3

3) Determine the mass of the metal inside the unit cell:

11.9 g cm^{-3} times 5.94665 x 10^{-23} cm^3 = 7.0765 x 10^{-22} g

3) The above mass is that of 4 atoms (based on our knowledge that the unit cell is fcc). Scale the mass to that of Avogadro Number of atoms:

7.0765 x 10^{-22} g is to 4 atoms as x is to 6.022 x 10^{23} atoms/mole

x = 106.5 g/mol

The metal is palladium.

Problem #14: Nickel oxide (NiO) crystallizes in the NaCl type of crystal structure. The length of the unit cell of NiO is 4.20 Å. Calculate the density of NiO.

Solution:

1) A brief discussion . . .

. . . of the NaCl structure is found here. Ignore the question and the last half of the answer.

The key point is that in the NaCl unit cell, there are 4 Na^+ and 4 Cl^-. You can think of it as a face-centered unit cell of chloride ions has been interpenetrated with a face-centered unit cell of sodium ions.

Following the above, a unit cell of NiO will contain 4 Ni^{2+} and 4 O^{2-}

2) Convert Å to cm:

1 Å = 10^{-8} cm (Ångströn is an old unit but still used from time to time)

4.20 Å = 4.20×10^{-8} cm

3) The volume of one NiO unit cell is this:

$(4.20 \times 10^{-8}\text{ cm})^3 = 7.4088 \times 10^{-23}\text{ cm}^3$

4) The weight of four NiO in the unit cell:

$(74.692\text{ g/mol} / 6.022 \times 10^{23}\text{ mol}^{-1}) \times 4 = 4.96128 \times 10^{-22}\text{ g}$

5) Determine the density:

$4.96128 \times 10^{-22}\text{ g} / 7.4088 \times 10^{-23}\text{ cm}^3 = 6.70\text{ g/cm}^3$

This compares to the book value of 6.67 g/cm^3

Problem #15: NiO adopts the face-centered-cubic arrangement. Given that the density of NiO is 6.67 g/cm^3, calculate the length of the edge of its unit cell (in pm).

Solution:

1) Calculate the average mass of one NiO formula unit:

74.692 g/mol divided by $6.022 \times 10^{23}\text{ mol}^{-1} = 1.24032 \times 10^{-22}\text{ g}$

2) NiO has the NaCl structure, so 4 Ni and 4 O per unit cell. Determine the total mass of NiO in one unit cell:

1.24032×10^{-22} g x 4 = 4.96128×10^{-22} g

3) Determine the volume of the unit cell:

4.96128×10^{-22} g divided by 6.67 g/cm^3 = 7.4382×10^{-23} cm^3

4) Determine the edge length:

7.4382×10^{-23} cm^{3}3 = 4.2055×10^{-8} cm

5) Convert from cm to pm:

4.2055×10^{-8} cm times (10^{10} pm / 1 cm) = 420.55 pm

A value of 420. pm seems reasonable as a final answer.
