Body-centered cubic problems

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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.

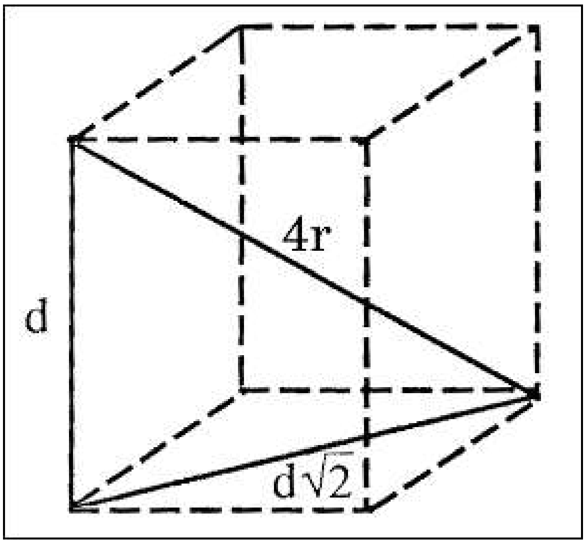
Solution:

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:

1.726868×10^{-22} g / 2.4056×10^{-23} cm^3 = 7.18 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:

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

$3d^2 = 802816$

$d^2 = 267605.3333\ldots$

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 x 10^{23} mol^{-1} = 3.81767 x 10^{-23} g (this is the average mass of one atom of Na)

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

2) Determine the volume of the unit cell:

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

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

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

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

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

$3d^2 = 16r^2$

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

d = 4.11 x 10^{-8} cm

3) Calcuate the volume of the unit cell:

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

4) Calcuate the mass inside the unit cell:

$6.95 \times 10^{-23}\ \text{cm}^3$ times $4.253\ \text{g/cm}^3 = 2.95 \times 10^{-22}$ 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 $6.022 \times 10^{23}\ \text{mol}^{-1}$

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 $10.28\ \text{g /cm}^3$.

Solution:

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

95.96 g/mol divided by $6.022 \times 10^{23}\ \text{mol}^{-1} = 1.59349 \times 10^{-22}$ 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 $10.28\ \text{g/cm}^3 = 3.100175 \times 10^{-23}\ \text{cm}^3$

3) Determine the edge length:

$3.100175 \times 10^{-23}\ \text{cm}^3 3 = 3.14144 \times 10^{-8}$ 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.

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

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

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

Cube the edge length to give the volume:

$2.7689 \times 10^{-23}\ cm^3$

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 $6.022 \times 10^{23}\ mol^{-1} = 8.459 \times 10^{-23}$ 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.

$1.6918 \times 10^{-22}\ g / 2.7689 \times 10^{-23}\ cm^3 = 6.11\ g/cm^3$

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

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

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

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

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

$3.53275 \times 10^{-23}\ cm^3$

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

3.28×10^{-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.

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

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

$16r^2 = 3d^2$

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

$r = d3 / 4$

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

$r = 1.42 \times 10^{-8}\ cm = 142\ pm$

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?

$(3.05 \text{ Å})^3 = 28.372625 \text{ Å}^3$

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?

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

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?

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

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

$19.26816686 \text{ Å}^3 / 28.372625 \text{ Å}^3 = 0.679$

67.9%

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Face-centered cubic problems

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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:

$106.42\ g\ mol^{-1} \div 6.022 \times 10^{23}$ atoms $mol^{-1} = 1.767187 \times 10^{-22}$ g/atom

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

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

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

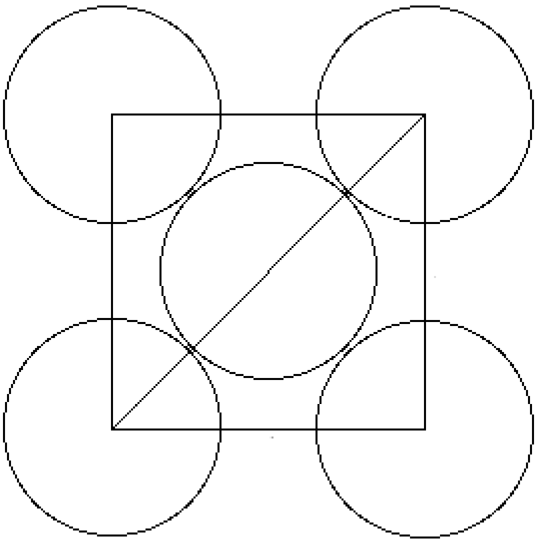
$7.068748 \times 10^{-22}\ g \div 12.023\ g/cm^3 = 5.8793545 \times 10^{-23}\ cm^3$

4) Determine the edge length of the unit cell:

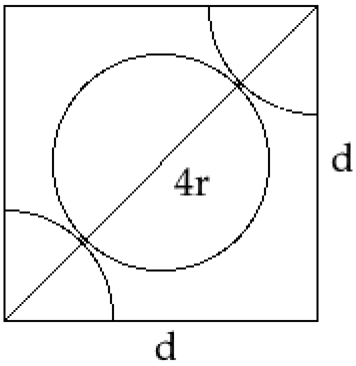
$5.8793545 \times 10^{-23}\ cm^3 3 = 3.88845 \times 10^{-8}$ cm

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:

$58.6934 \text{ g mol}^{-1} \div 6.022 \times 10^{23} \text{ atoms mol}^{-1} = 9.746496 \times 10^{-23}$ g/atom

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

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

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

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

4) Determine the edge length of the unit cell:

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

5) Convert cm to pm:

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

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

(3.524×10^{-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) = 1.97×10^{-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:

(5.572×10^{-8} cm)^3 = 1.730×10^{-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 6.022×10^{23} atoms/mol = 6.6556×10^{-23} g/atom

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

5) Determine density:

2.66224×10^{-22} g divided by 1.730×10^{-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) = 559×10^{-10} cm = 5.59×10^{-8} cm

2) Calculate the volume of the unit cell:

$(5.59 \times 10^{-8}\ \text{cm})^3 = 1.7468 \times 10^{-22}\ \text{cm}^3$

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

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

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

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

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

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

Solution to b:

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

$r = d \div \sqrt{8}$ <--- one of two alternate formulations

$r = 5.59 \times 10^{-8}\ \text{cm} \div \sqrt{8}$

$r = 1.98 \times 10^{-8}$ 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:

3.23×10^{-23} cm^3 times 4 = 1.29×10^{-22} cm^3

2) Calculate volume of cell not filled with Kr:

1.7468×10^{-22} cm^3 minus 1.29×10^{-22} cm^3 = 4.568×10^{-23} cm^3

3) Calculate % empty space:

4.568×10^{-23} cm^3 divided by 1.7468×10^{-22} 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:

4.06×10^{-10} m = 4.06×10^{-8} cm

2) Determine the volume of the unit cube:

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

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

11.5 g/cm^3 times 6.69234×10^{-23} cm^3 = 7.696193×10^{-22} 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):

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

1.97×10^{-8} cm = $d \div 2(\sqrt{2})$

$d = 5.572 \times 10^{-8}$ cm

3) Determine the volume of the unit cell:

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

4) Determine grams of metal in unit cell:

$1.72995 \text{ x } 10^{-22} \text{ cm}^3$ times $1.54 \text{ g/cm}^3 = 2.6641 \text{ x } 10^{-22}$ g

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

$2.6641 \text{ x } 10^{-22}$ g is to 4 atoms as x grams is to $6.022 \text{ x } 10^{23}$ 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) = $2.15 \text{ x } 10^{-8}$ 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

$2.15 \text{ x } 10^{-8}$ cm = d ÷ √8

d = $6.08112 \text{ x } 10^{-8}$ cm

3) Determine the volume of the unit cell:

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

4) Determine grams of metal in unit cell:

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

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

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

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

$2L^2 = 4d^2$

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

$L / 2^{1/2} = d$

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 x 10^{-8} cm

(3.833 x 10^{-8} cm)^3 = 5.6314 x 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 x 10^{-23} cm^3 = 1.27326 x 10^{-21} g

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

1.27326 x 10^{-21} g divided by 192.217 g/mol = 6.624075 x 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 x 10^{-24} mol as x is to 1.000 mol

x = 6.038 x 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 x 10^{-8} cm)^3 = 6.0698 x 10^{-23} cm^3

Determine the mass of Pt in the unit cell:

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

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

$r = 1.39 \times 10^{-8}$ 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 $(1 \text{ m} / 10^{12} \text{ pm}) = 392.0 \times 10^{-12} \text{ m} = 3.920 \times 10^{-10}$ 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 $6.022 \times 10^{23} \text{ mol}^{-1} = 3.239422 \times 10^{-22}$ 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:

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

The book value is $21450 \text{ kg} / \text{m}^3$.

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:

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

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)

$4.20 \text{ Å} = 4.20 \times 10^{-8}$ 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:

$(74.692 \text{ g/mol} / 6.022 \times 10^{23} \text{ mol}^{-1}) \times 4 = 4.96128 \times 10^{-22}$ 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 $6.022 \times 10^{23} \text{ mol}^{-1} = 1.24032 \times 10^{-22}$ 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:

$1.24032 \times 10^{-22} \text{ g} \times 4 = 4.96128 \times 10^{-22}$ g

3) Determine the volume of the unit cell:

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

4) Determine the edge length:

$7.4382 \times 10^{-23} \text{ cm}^3 3 = 4.2055 \times 10^{-8}$ 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.

Go to a list of only the problems

Go to some body-centered cubic problems

Go to some general unit cell problems

Return to the Liquids & Solids menu

If the atomic radius of lead is 0.175 nm, calculate the volume of its unit cell in cubic meters

4.1 For this problem, we are asked to calculate the volume of a unit cell of lead. Lead has an FCC crystal structure (Table 4.1). The FCC unit cell volume may be computed from Equation 4.4 as

$$V_C = 16R^3\sqrt{2} = (16)(0.175 \times 10^{-9}\ \text{m})^3(\sqrt{2}) = 1.213 \times 10^{-28}\ \text{m}^3$$

Molybdenum has a BCC crystal structure, an atomic radius of 0.1363 nm, and an atomic weight of 95.94 g/mol. Compute its density.

4.6 This problem calls for a computation of the density of molybdenum. According to Equation 4.5

$$\rho = \frac{nA_{\text{Mo}}}{V_C N_{\text{A}}}$$

For BCC, n = 2 atoms/unit cell, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 \qquad \rho = \frac{nA_{\text{Mo}}}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_{\text{A}}}$$

Thus, $$= \frac{(2\ \text{atoms/unit cell})(95.94\ \text{g/mol})}{\left[(4)(0.1363 \times 10^{-7}\ \text{cm})^3/\sqrt{3}\right]^3/(\text{unit cell})(6.023 \times 10^{23}\ \text{atoms/mol})}$$

$$= 10.21\ \text{g/cm}^3$$

Calculate the radius of a palladium atom, given that Pd has an FCC crystal structure, a density of 12.0 g/cm^3, and an atomic weight of 106.4 g/mol.

4.7 We are asked to determine the radius of a palladium atom, given that Pd has an FCC crystal structure. For FCC, n = 4 atoms/unit cell, and $V_C = 16R^3\sqrt{2}$ (Equation 4.4). Now,

$$\rho = \frac{nA_{\text{Pd}}}{V_C N_{\text{A}}} = \frac{nA_{\text{Pd}}}{(16R^3\sqrt{2})N_{\text{A}}}$$

And solving for R from the above expression yields

$$R = \left(\frac{nA_{\text{Pd}}}{16\rho N_{\text{A}}\sqrt{2}}\right)^{1/3} = \left[\frac{(4\ \text{atoms/unit cell})(106.4\ \text{g/mol})}{(16)(12.0\ \text{g/cm}^3)(6.023 \times 10^{23}\ \text{atoms/mol})(\sqrt{2})}\right]^{1/3} = 1.38 \times 10^{-8}\ \text{cm} = 0.138\ \text{nm}$$

Calculate the radius of a tantalum atom, given that Ta has a BCC crystal structure, a density of 16.6 g/cm^3, and an atomic weight of 180.9 g/mol.

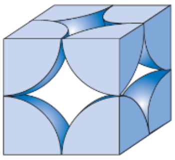
4.8 This problem asks for us to calculate the radius of a tantalum atom. For BCC, n = 2 atoms/unit cell, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

$$\rho = \frac{nA_{\mathrm{Ta}}}{V_C N_A} = \frac{nA_{\mathrm{Ta}}}{\left(\frac{64R^3}{3\sqrt{3}}\right)N_A}$$

$$R = \left(\frac{3\sqrt{3}nA_{\mathrm{Ta}}}{64\rho N_A}\right)^{1/3} = \left[\frac{(3\sqrt{3})\,(2\text{ atoms/unit cell})\,(180.9\text{ g/mol})}{(64)\left(16.6\text{ g/cm}^3\right)\left(6.023\text{ x }10^{23}\text{ atoms/mol}\right)}\right]^{1/3} = 1.43\text{ x }10^{-8}\text{ cm} = 0.143\text{ nm}$$

Some hypothetical metal has the simple cubic crystal structure shown in Figure. If its atomic weight is 74.5 g/mol and the atomic radius is 0.145 nm, compute its density.



4.9 For the simple cubic crystal structure, the value of n in Equation 4.5 is unity since there is only a single atom associated with each unit cell. Furthermore, for the unit cell edge length, $a = 2R$ (Figure 4.38). Therefore, employment of Equation 4.5 yields

$$\rho = \frac{nA}{V_C N_A} = \frac{nA}{(2R)^3 N_A} = \frac{(1\text{ atom/unit cell})(74.5\text{ g/mol})}{\left\{\left[(2)(1.45\text{ x }10^{-8}\text{ cm})\right]^3/(\text{unit cell})\right\}\left(6.023\text{ x }10^{23}\text{ atoms/mol}\right)} \quad 5.07\text{ g/cm}^3$$

Niobium has an atomic radius of 0.1430 nm and a density of 8.57 g/cm³. Determine whether it has an FCC or BCC crystal structure, the atomic weight of Niobium is 92.91 g/mol. which is the value provided in the problem statement. Therefore, Nb has a BCC crystal structure

4.12 In order to determine whether Nb has an FCC or a BCC crystal structure, we need to compute its density for each of the crystal structures. For FCC, $n = 4$, and $a = 2R\sqrt{2}$ (Equation 4.1). Also, from Figure 2.6, its atomic weight is 92.91 g/mol. Thus, for FCC (employing Equation 4.5)

$$\rho = \frac{nA_{\mathrm{Nb}}}{a^3 N_A} = \frac{nA_{\mathrm{Nb}}}{(2R\sqrt{2})^3 N_A} = \frac{(4\text{ atoms/unit cell})(92.91\text{ g/mol})}{\left\{\left[(2)(1.43\times10^{-8}\text{ cm})(\sqrt{2})\right]^3/(\text{unit cell})\right\}(6.023\times10^{23}\text{ atoms/mol})} = 9.33\text{ g/cm}^3$$

For BCC, $n = 2$, and $a = \frac{4R}{\sqrt{3}}$ (Equation 4.3), thus

$$\rho = \frac{nA_{\mathrm{Nb}}}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_A} \quad \rho = \frac{(2\text{ atoms/unit cell})(92.91\text{ g/mol})}{\left\{\left[\frac{(4)(1.43\times10^{-8}\text{ cm})}{\sqrt{3}}\right]^3/(\text{unit cell})\right\}(6.023\times10^{23}\text{ atoms/mol})} = 8.57\text{ g/cm}^3$$

The unit cell for uranium has orthorhombic symmetry, with *a*, *b*, and *c* lattice parameters of 0.286, 0.587, and 0.495 nm, respectively. If its density, atomic weight, and atomic radius are 19.05 g/cm^3, 238.03 g/mol, and 0.1385 nm, respectively, compute the atomic packing factor.

4.14 In order to determine the APF for U, we need to compute both the unit cell volume (V_C) which is just the product of the three unit cell parameters, as well as the total sphere volume (V_S) which is just the product of the volume of a single sphere and the number of spheres in the unit cell (n). The value of n may be calculated from Equation 4.5 as

$$n = \frac{\rho V_C N_A}{A_U} = \frac{(19.05\ \text{g/cm}^3)(2.86)(5.87)(4.95)(\times 10^{-24}\ \text{cm}^3)(6.023 \times 10^{23}\ \text{atoms/mol})}{238.03\ \text{g/mol}} = 4.01\ \text{atoms/unit cell}$$

Therefore

$$\text{APF} = \frac{V_S}{V_C} = \frac{(4)\left(\frac{4}{3}\pi R^3\right)}{(a)(b)(c)} = \frac{(4)\left[\frac{4}{3}(\pi)(1.385\text{Ź}x\ 10^{8}\ \text{cm})^3\right]}{(2.86)(5.87)(4.95)(x\text{Ź}10^{24}\ \text{cm}^3)} = 0.536$$

Determine the total void volume (cm^3 /mole) for gold (Au) at 27^{o}C; make the hard-sphere approximation in your calculation, and use data provided in the periodic table.

First determine the packing density for Au, which is FCC; then relate it to the molar volume given in the periodic table.

$$\text{packing density} = \frac{\text{volume of atoms/unit cell}}{\text{volume of unit cell}} = \frac{\frac{16\pi r^3}{3}}{a^3} = \frac{16\pi r^3}{3a^3}$$

$$\text{packing density} = \frac{16\pi r^3}{3 \times 16\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}} = 0.74 = 74\%$$

$$\text{void volume} = 1 - \text{packing density} = 26\%$$

From the packing density (74%) we recognize the void volume to be 26%. Given the molar volume as 10.3 cm^3/mole, the void volume is:

$$0.26 \times 10.3\ \text{cm}^3/\text{mole} = 2.68\ \text{cm}^3/\text{mole}$$

Determine the atomic radius of Mo. Given that atomic weight is 95.94 g/mol and density of Mo is 10.2 g/cm^3.

Mo: atomic weight = 95.94 g/mole

ρ = 10.2 g/cm^3

BCC, so n = 2 atoms/unit cell

$$a^3 = \frac{(95.94 \text{ g/mole})(2 \text{ atoms/unit cell})}{(10.2 \text{ g / cm}^3)(6.023 \times 10^{23} \text{ atoms/mole})} \times 10^{-6} \frac{\text{m}^3}{\text{cm}^3}$$

$$= 3.12 \times 10^{-29} \text{ m}^3$$

$$a = 3.22 \times 10^{-10} \text{ m}$$

For BCC, $a\sqrt{3} = 4r$, so $r = 1.39 \times 10^{-10}$ m

A metal is found to have BCC structure, a lattice constant of 3.31 Angstroms, and a density of 16.6 g/cm^3. Determine the atomic weight of the element.

BCC structure, so n = 2

a = 3.31 Å = 3.31 x 10^{-10} m

ρ = 16.6 g/cm^3

$$\frac{\text{atomic weight}}{\rho} \times 10^{-6} = \frac{N_A}{n} \times a^3$$

$$\text{atomic weight} = \frac{(6.023 \times 10^{23} \text{ atoms/mole})\,(3.31 \times 10^{-10} \text{ m})^3}{(2 \text{ atoms/unit cell})(10^{-6} \text{ m}^3/\text{cm}^3)} \times 16.6 \text{ g/cm}^3$$

$$= 181.3 \text{ g/mole}$$

Session #15: Homework Solutions

Problem #1

Iron ($\rho = 7.86\ g/cm^3$) crystallizes in a BCC unit cell at room temperature. Calculate the radius of an iron atom in this crystal. At temperatures above 910ºC iron prefers to be FCC. If we neglect the temperature dependence of the radius of the iron atom on the grounds that it is negligible, we can calculate the density of FCC iron. Use this to determine whether iron expands or contracts when it undergoes transformation from the BCC to the FCC structure.

Solution

In BCC there are 2 atoms per unit cell, so $\frac{2}{a^3} = \frac{N_A}{V_{molar}}$, where $V_{molar} = A/\rho$; A is the atomic mass of iron.

$$\frac{2}{a^3} = \frac{N_A \times \rho}{A}$$

$$\therefore\ a = \left(\frac{2A}{N_A \times \rho}\right)^{\frac{1}{3}} = \frac{4}{\sqrt{3}} r$$

$$\therefore\ r = 1.24 \times 10^{-8}\ cm$$

If we assume that change of phase does not change the radius of the iron atom, then we can repeat the calculation in the context of an FCC crystal structure, i.e., 4 atoms per unit cell and $a = 2\sqrt{2}r$.

$$\rho = \frac{4A}{N_A (2\sqrt{2}r)^3} = 8.60\ g/cm^3$$

FCC iron is more closely packed than BCC suggesting that iron contracts upon changing from BCC to FCC. This is consistent with the packing density calculations reported in lecture that give FCC as being 74% dense and BCC 68% dense. The ratio of the densities calculated here is precisely the same:

$$\frac{7.86}{8.60} = \frac{0.68}{0.74}$$

Problem #2

Determine the total void volume (cm^3/mole) for gold (Au) at 27ºC; make the hard-sphere approximation in your calculation, and use data provided in the periodic table.

Solution

First determine the packing density for Au, which is FCC; then relate it to the molar volume given in the periodic table.

$$\text{packing density} = \frac{\text{volume of atoms/unit cell}}{\text{volume of unit cell}} = \frac{\frac{16\pi r^3}{3}}{a^3} = \frac{16\pi r^3}{3a^3}$$

$$\text{packing density} = \frac{16\pi r^3}{3 \times 16\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}} = 0.74 = 74\%$$

$$\text{void volume} = 1 - \text{packing density} = 26\%$$

From the packing density (74%) we recognize the void volume to be 26%. Given the molar volume as 10.3 cm^3/mole, the void volume is:

$$0.26 \times 10.3\ cm^3/\text{ mole} = 2.68\ cm^3\ /\text{ mole}$$

Problem #3

Determine the atomic (metallic) radius of Mo. Do not give the value listed in the periodic table; calculate it from other data given.

Solution

Mo: atomic weight = 95.94 g/mole

ρ = 10.2 g/cm^3

BCC, so n = 2 atoms/unit cell

$$a^3 = \frac{(95.94\text{ g/mole})(2\text{ atoms/unit cell})}{(10.2\text{ g / cm}^3)(6.023 \times 10^{23}\text{ atoms/mole})} \times 10^{-6}\ \frac{m^3}{cm^3}$$

$$= 3.12 \times 10^{-29}\ m^3$$

$$a = 3.22 \times 10^{-10}\ m$$

For BCC, $a\sqrt{3} = 4r$, so $r = 1.39 \times 10^{-10}$ m

Problem #4

A metal is found to have BCC structure, a lattice constant of 3.31 Å, and a density of 16.6 g/cm^3. Determine the atomic weight of this element.

Solution

BCC structure, so n = 2

a = 3.31 Å = 3.31 x 10^{-10} m

ρ = 16.6 g/cm^3

$$\frac{\text{atomic weight}}{\rho} \times 10^{-6} = \frac{N_A}{n} \times a^3$$

$$\text{atomic weight} = \frac{(6.023 \times 10^{23}\ \text{atoms/mole})\ (3.31 \times 10^{-10}\ \text{m})^3}{(2\ \text{atoms/unit cell})(10^{-6}\ \text{m}^3/\text{cm}^3)} \times 16.6\ \text{g/cm}^3$$

$$= 181.3\ \text{g/mole}$$

Problem #5

At 100°C copper (Cu) has a lattice constant of 3.655 Å. What is its density at this temperature?

Solution

Cu is FCC, so n = 4

$a = 3.655$ Å $= 3.655 \times 10^{-10}$ m

atomic weight = 63.55 g/mole

$$\frac{\text{atomic weight}}{\rho} \times 10^{-6} = \frac{N_A}{n} \times a^3$$

$$\rho = \frac{(63.55\ \text{g/mole})(4\ \text{atoms/unit cell})}{(6.023 \times 10^{23}\ \text{atoms/mole})(3.655 \times 10^{-10}\ \text{m}^3)} = 8.64\ \text{g/cm}^3$$

Problem #6

Determine the second-nearest neighbor distance for nickel (Ni) (in pm) at 100° C if its density at that temperature is 8.83 g/cm^3.

Solution

Ni: n = 4

atomic weight = 58.70 g/mole

$\rho = 8.83\ \text{g/cm}^3$

For a face−centered cubic structure, the second nearest neighbor distance equals "a" (see LN4−11).

$$\frac{\text{atomic weight}}{\rho} \times 10^{-6} = \frac{N_A}{n} \times a^3$$

$$a^3 = \frac{(58.70\ \text{g/mole})(10^{-6}\ \text{m}^3/\text{cm}^3)(4\ \text{atoms /unit cell})}{(6.023 \times 10^{23}\ \text{atoms / mole})(8.83\ \text{g / cm}^3)}$$

$$= 4.41 \times 10^{-29}\ \text{m}^3$$

$$a = 3.61 \times 10^{-10}\ \text{m} \times \frac{10^{12}\ \text{pm}}{\text{m}} = 3.61 \times 10^2\ \text{pm}$$

Problem #7

Determine the highest linear density of atoms (atoms/m) encountered in vanadium (V).

Solution

V: atomic weight = 50.94 g/mole

$\rho = 5.8\ g/cm^3$

BCC, so n = 2

The highest density would be found in the [111] direction. To find "a":

$$\frac{\text{atomic weight}}{\rho} = a^3 \frac{N_A}{n} \rightarrow a^3 = \frac{50.94 \times 2}{5.8 \times 6.023 \times 10^{23}}$$

$a = 3.08 \times 10^{-8}$ cm $= 3.08 \times 10^{-10}$ m

The length in the [111] direction is $a\sqrt{3}$, so there are:

2 atoms / $a\sqrt{3}$ = 2 atoms/(3.08×10^{-10} m $\times \sqrt{3}$)

= 3.75×10^9 atoms/m

3.091SC Introduction to Solid State Chemistry
Fall 2009

General unit cell problems

Go to the body-centered cubic problems

Go to the face-centered cubic problems

Return to the Liquids & Solids menu

Problem #1: Many metals pack in cubic unit cells. The density of a metal and length of the unit cell can be used to determine the type for packing. For example, sodium has a density of 0.968 g/cm^3 and a unit cell side length (a) of 4.29 Å

a. How many sodium atoms are in 1 cm^3?
b. How many unit cells are in 1 cm^3?
c. How many sodium atoms are there per unit cell?

Solution:

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

$$22.99 \text{ g mol}^{-1} \div 6.022 \times 10^{23} \text{ atoms mol}^{-1} = 3.82 \times 10^{-23} \text{ g/atom}$$

2) Determine atoms in 1 cm^3:

$$0.968 \text{ g} / 3.82 \times 10^{-23} \text{ g/atom} = 2.54 \times 10^{22} \text{ atoms in 1 cm}^3$$

3) Determine volume of the unit cell:

$$(4.29 \times 10^{-8} \text{ cm})^3 = 7.89 \times 10^{-23} \text{ cm}^3$$

4) Determine number of unit cells in 1 cm^3:

$$1 \text{ cm}^3 / 7.89 \times 10^{-23} \text{ cm}^3 = 1.27 \times 10^{22} \text{ unit cells}$$

5) Determine atoms per unit cell:

$$2.54 \times 10^{22} \text{ atoms} / 1.27 \times 10^{22} \text{ unit cells} = 2 \text{ atoms per unit cell}$$

Problem #2: Metallic iron crystallizes in a type of cubic unit cell. The unit cell edge length is 287 pm. The density of iron is 7.87 g/cm3. How many iron atoms are there within one unit cell?

Solution:

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

$$55.845 \text{ g mol}^{-1} \div 6.022 \times 10^{23} \text{ atoms mol}^{-1} = 9.2735 \times 10^{-23} \text{ g/atom}$$

2) Determine atoms in 1 cm^3:

$$7.87 \text{ g} / 9.2735 \times 10^{-23} \text{ g/atom} = 8.4866 \times 10^{22} \text{ atoms in 1 cm}^3$$

3) Determine volume of the unit cell:

$$287 \text{ pm} \times (1 \text{ cm} / 10^{10} \text{ pm}) = 2.87 \times 10^{-8} \text{ cm}$$

$(2.87 \times 10^{-8}\ cm)^3 = 2.364 \times 10^{-23}\ cm^3$

4) Determine number of unit cells in 1 cm^3:

$1\ cm^3 / 2.364 \times 10^{-23}\ cm^3 = 4.23 \times 10^{22}$ unit cells

5) Determine atoms per unit cell:

8.4866×10^{22} atoms / 4.23×10^{22} unit cells = 2 atoms per unit cell

---

Problem #3: (a) You are given a cube of silver metal that measures 1.015 cm on each edge. The density of silver is 10.49 g/cm^3. How many atoms are in this cube?

Solution to a:

$(1.015\ cm)^3 \times (10.49\ g / cm^3) \times (1\ mole\ Ag / 107.9\ g) \times (6.023 \times 10^{23}\ atoms / 1\ mole) = 6.12 \times 10^{22}$ atoms Ag

(b) Because atoms are spherical, they cannot occupy all of the space of the cube. The silver atoms pack in the solid in such a way that 74% of the volume of the solid is actually filled with the silver atoms. Calculate the volume of a single silver atom.

Solution to b:

$(1.015\ cm)^3 \times 0.74 = 0.774\ cm^3$ filled by Ag atoms
$0.774\ cm^3 / (6.12 \times 10^{22}\ atoms) = 1.26 \times 10^{-23}\ cm^3$ / Ag atom

(c) Using the volume of a silver atom and the formula for the volume of a sphere, calculate the radius in angstroms of a silver atom.

Solution to c:

$V = (4/3)\ \pi\ r^3$
$r^3 = V / (4/3)\ \pi = [(1.26 \times 10^{-23}\ cm^3)\ (3)] / [(4)\ (3.14159)] = 3.008 \times 10^{-24}\ cm^3$

$r = 1.4435 \times 10^{-8}\ cm = 1.44$ Å

Problem #4: Many metals pack in cubic unit cells. The density of a metal and length of the unit cell can be used to determine the type for packing. For example, gold has a density of 19.32 g/cm^3 and a unit cell side length of 4.08 Å. (1 Å = 1×10^{-8} cm.)

(a) How many gold atoms are in exactly 1 cm^3?
(b) How many unit cells are in exactly 1 cm^3?
(c) How many gold atoms are there per unit cell?
(d) The atoms/unit cell suggests that gold packs as a (i) simple, (ii) body-centered or (iii) face-centered unit cell.

Solution:

1) Part a:

19.32 g / 197.0 g/mol = 0.098071 mol

0.098071 mol times 6.022×10^{23} atoms/mol = 5.9058×10^{22} atoms

2) Part b:

4.08 Å = 4.08×10^{-8} cm

1 cm divided by 4.08×10^{-8} cm = 24509804 (this is how many 4.08 Å segments in 1 cm)

24509804 cubed = 1.47238×10^{22} unit cells

3) Part c:

5.9058×10^{22} atoms / 1.47238×10^{22} unit cells = 4 atom/unit cell

4) Part d:

face-centered

Problem #5: A metal nitride has a nitrogen atom at each corner and a metal atom at each edge. Which is the empirical formula for this nitride?

a. Ba_3N_2
b. Na_3N
c. AlN
d. Ti_3N_4

Solution:

A cube has eight corners and an atom at a corner is in eight different cubes; therefore 1/8 of an atom at each corner of a given cube. So:

1/8 times 8 = 1 total nitrogen atom in each cube

A cube has 12 edges and each edge is in 4 different cubes, so there is 1/4 of an atom in each individual cube. So:

1/4 times 12 = 3 total metal atoms in each cube

The only choice to fit the above criteria is answer choice b, Na_3N.

Problem #6: Calcium fluoride crystallizes with a cubic lattice. The unit cell has an edge of 546.26 pm and has a density of 3.180 g/cm^3. How many formula units must there be per unit cell?

Solution:

1) Convert pm to cm:

546.26 pm times (1 cm / 10^{10} pm) = 5.4626×10^{-8} cm

2) Determine volume of unit cell:

$(5.4626 \times 10^{-8} \text{ cm})^3 = 1.63 \times 10^{-22} \text{ cm}^3$

3) Determine mass of CaF_2 in unit cell:

3.180 g/cm^3 times 1.63×10^{-22} cm^3 = 5.1835×10^{-22} g

4) Determine mass of one formula unit of CaF_2:

formula weight of CaF_2 = 78.074 g/mol

78.074 g/mol divided by 6.022×10^{23} formula units / mole = 1.2965×10^{-22} g

5) Determine number of formula units in one unit cell:

5.1835×10^{-22} g divided by 1.2965×10^{-22} g = 3.998

There are 4 formula units of CaF_2 per unit cell

Problem #7: Tungsten has an atomic radius of 137 pm and crystallizes in a cubic unit cell having an edge length d = 316 pm. What type of cubic unit cell does tungsten crystallize in?

Solution:

Let us assume the cell is face-centered. If this is the case, then this relationship should hold true:

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

where r = the radius.

Please see a small discussion of this in problem #1 here.

Using 316 pm for d and 548 pm for 4r, we have this:

$316^2 + 316^2$?=? 548^2

We find 199712 for the left and 300304 for the right, so the idea that tungsten is fcc fails.

For body-centered, please see problem #2 here for this equation:

$d^2 + (d\sqrt{2})^2 = (4r)^2$

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

$3(316^2)$?=? 548^2

299568 = 300304

Due to the fact that these numbers are roughly equivalent, we can conclude that tungsten is being body-centered cubic.

Problem #8: What is the formula of the compound that crystallizes with Ba^{2+} ions occupying one-half of the cubic holes in a simple cubic arrangement of fluoride ions?

Solution:

We must consider two cubic unit cells, one with the barium ion and one without (this gives us one-half of the cubic holes filled).

Cell 1: 8 F atoms at the 8 vertices. Since each vertex is in a total of 8 cells, we have 1 F atom in the unit cell. The cubic hole in the middle of the cell is empty.

Cell 2: 8 F atoms at the 8 vertices. Since each vertex is in a total of 8 cells, we have 1 F atom in the unit cell. The cubic hole in the middle of the cell has a barium in it.

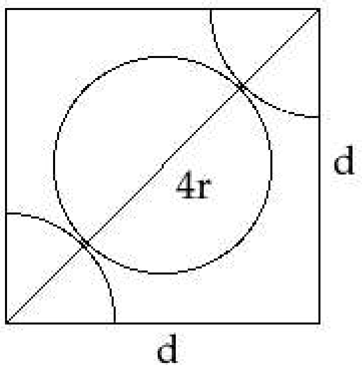
Total for the two cells: one Ba and two F

Formula: BaF_2

Problem #9: The radius of gold is 144 pm, and the density is 19.32 g/cm^3. Does gold crystallize in a face-centered cubic structure or a body-centered cubic structure?

Solution:

1) I will assume the unit cell is face-centered cubic. I will use that assumption and the atomic radii to calculate the volume of the cell. From there, I will use the fact that there are 4 atoms of gold in the unit cell to determine the density. The final step will be to compare it to the 19.32 value. Here is one face of a face-centered cubic unit cell:



2) Across the face of the unit cell, there are 4 radii of gold, hence 576 pm. Using the Pythagorean Theorem, we determine the edge length of the unit cell:

$d^2 + d^2 = 576^2$

d = 407.2935 pm

3) Let us convert the pm to cm:

4407.2935 pm times (1 cm / 10^{10} pm) = 4.072935×10^{-8} cm

4) The volume of the unit cell:

$(4.072935 \times 10^{-8}\ \text{cm})^3 = 6.75651 \times 10^{-23}\ \text{cm}^3$

5) The mass of 4 gold atoms:

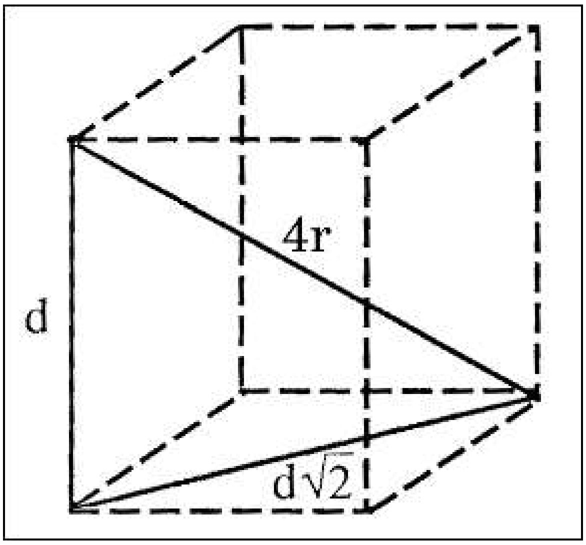
(196.96655 g/mol divided by 6.022×10^{23} atoms/mol) times 4 atoms = 1.308313×10^{-21} g

6) Let's see what density results:

$1.308313 \times 10^{-21}\ \text{g} / 6.75651 \times 10^{-23}\ \text{cm}^3 = 19.36\ \text{g/cm}^3$

We conclude that gold crystallizes fcc because we were able to reproduce the known density of gold.

7) Let's do the bcc calculation (which we know will give us the wrong answer). Here's an image showing what to do with the Pythagorean Theorem:



8) The rest of the calculation with minimal comment:

$d^2 + (d\sqrt{2})^2 = 576^2$

d = 332.55 pm

332.55 pm = 3.3255×10^{-8} cm

$(3.3255 \times 10^{-10}\text{ cm})^3 = 3.6776 \times 10^{-23}\text{ cm}^3$

There are two atoms in a body-centered cubic.

(197 g/mol divided by 6.022×10^{23} atoms/mol) times 2 atoms = 6.5427×10^{-22} g

6.5427×10^{-22} g / 3.6776×10^{-23} cm^3 = 17.79 g/cm^3

Gold does not crystallize bcc because bcc does not reproduce the known density of gold.

Problem #10: Avogadro's number has been determined by about 20 different methods. In one approach, the spacing between ions in an ionic substance is determined by using X-ray diffraction. X-ray diffraction of sodium chloride have shown that the distance between adjacent Na^+ and Cl^- ions is 2.819×10^{-8} cm. The density of solid NaCl is 2.165 g/cm^3. By calculating the molar mass to four significant figures, you can determine Avogadro's number. What value do you obtain?

Solution:

1) Imagine a cube with 4 Na and 4 Cl at adjacent vertices. I'll call it the reference cube.

There's going to be a twist and it involves how many Na and Cl are in the cube. Think about it before the reveal in the last step.

2) Determine the volume of the cube:

$(2.819 \times 10^{-8}\text{ cm})^3 = 2.2402 \times 10^{-23}\text{ cm}^3$

3) Calculate the mass of NaCl inside the cube:

2.2402×10^{-23} cm^3 times 2.165 g/cm^3 = 4.85×10^{-23} g

4) The molar mass divided by the mass inside the cube equals Avogadro's Number. Here's where the twist comes into play.

Each Na and each Cl at a vertex of the reference cube is shared by a total of 8 cubes. (You may verify this on your own.) At any one vertex, there is 1/8 of a Na atom and 1/8 of a Cl atom inside the reference cube.

With the reference cube having 4 vertices of Na and 4 vertices of Cl, this means there is a total of 1/2 of a Na atom and 1/2 of a Cl atom inside the reference cube.

The "molar mass" of (1/2)NaCl is half of 58.443.

29.2215 g/mol divided by 4.85×10^{-23} g = 6.025×10^{23} mol^{-1}

Problem #11: Many metals pack in cubic unit cells. The density of a metal and length of the unit cell can be used to determine the type for packing. For example, platinum has a density of 21.45 g/cm^3 and a unit cell side length a of 3.93 Å. What is the atomic radius of platinum?

Solution:

1) Determine the volume of the unit cell:

$(3.93 \times 10^{-8}$ cm$)^3 = 6.07 \times 10^{-23}$ cm^3

Note that I converted from Å to cm. That's because of the density.

2) Determine the mass of Pt in one unit cell:

6.07×10^{-23} cm^3 times 21.45 g/cm^3 = 1.302×10^{-21} g

3) Determine number of Pt atoms in the given mass:

195.078 g/mol divided by 6.022 x 10^23 atom/mol = 3.2394×10^{-22} g/atom

1.302×10^{-21} g divided by 3.2394×10^{-22} g/atom = 4 atoms

I did the above calculations in order to determine if the unit cell was face-centered or body-centered. The answer of 4 atoms in the unit cell tells me that it is face-centered. I now know what to do to determine the atomic radius. To do so, I will use the Pythagorean Theorem. (See Problem #9 for an image illustrating a face-centered cubic.)

4) Solve the Pythagorean Theorem:

$d^2 + d^2 = (4r)^2$ (where r is the radius of the Pt atom. Four of them span the hypotenuse.)

$3.93^2 + 3.93^2 = 16r^2$

$r^2 = 30.8898 / 16 = 1.9306125$

r = 1.39 Å

Problem #12: The density of TlCl(s) is 7.00 g/cm^3 and that the length of an edge of a unit cell is 385 pm, (a) determine how many formula units of TlCl there are in a unit cell. Based on your answer for the number of formula units of TlCl(s) in a unit cell, (b) how is the unit cell of TlCl(s) likely to be structured?

Solution to (a):

1) Get the volume in cm:

(385 pm) (100 cm / 10^{12} pm) = 3.85 x 10^{-8} cm

2) Calculate the volume of the unit cell:

(3.85 x 10^{-8} cm)^3 = 5.7066625 x 10^{-23} cm^3

3) Calculate the mass of TlCl in one unit cell:

(7.00 g/cm^3) (5.7066625 x 10^{-23} cm^3) = 3.99466375 x 10^{-22} g

4) Determine how many moles of TlCl are in the unit cell:

3.99466375 x 10^{-22} g / 239.833 g/mol = 1.6656022107 x 10^{-24} mol

5) Formula units of TlCl in the unit cell:

(1.6656022107 x 10^{-24} mol) (6.022 x 10^{23} mol^{-1}) = 1.00

Solution to (b):

Body-centered cubic has two atoms per unit cell and a formula unit of TlCl has two atoms. One atom, say the chloride ion, occupies the center of the unit cell, while 1/8th of eight Tl^+ ions are present at each of the 8 vertices of the cube.

Face-centered cubic has 4 atoms per unit cell. The distribution of TlCl formula units into an fcc cell does not work.

Go to the body-centered cubic problems

Go to the face-centered cubic problems

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