CH 222 Winter 2025:
"Linear Regression & The Crystal Structures of Solids
*(online)" **Lab** - Instructions*

Note: **This is the lab for section W1 of CH 222 only.**

- *If you are taking section 01 or section H1 of CH 222*, please use this link:
  http://mhchem.org/r/6a.htm

Step One:

Watch the lab video for the "Linear Regression / Crystals" lab, found here:
http://mhchem.org/y/6.htm

Record the data found at the ***end*** of the lab video on page Ib-6-12.

Step Two:

Complete pages Ib-6-11 through Ib-6-16 using the "Linear Regression / Crystals" video and the actual lab instructions on pages Ib-6-2 through Ib-6-9.

Step Three:

Submit your lab (pages Ib-6-11 through Ib-6-16 *only* with computer generated graphs to avoid a point penalty**) as a *single* PDF file to the instructor via email (mike.russell@mhcc.edu) on Wednesday, February 19 by 11:59 PM.** I recommend a free program (ex: CamScanner, https://camscanner.com) or a website (ex: CombinePDF, https://combinepdf.com) to convert your work to a PDF file. Do ***not*** include graphs as separate file(s).... have all documents in one file to avoid a point penalty.

If you have any questions regarding this assignment, please email (mike.russell@mhcc.edu) the instructor! Good luck on this assignment!

Linear Regression & The Crystal Structures of Solids

This lab will demonstrate the power of a linear regression analysis while graphing linear data. We will also explore the techniques used to analyze several common types of metals in crystallography.

An **equation** is a mathematical model used to describe the relationship between variables. We will focus on **linear** equations in this lab which use a horizontal (X) axis (the **independent** variable, the variable we input when we make a measurement) and a vertical (Y) axis (the **dependent** variable, the number we measure after we set the X value.) If the plotted data points form a straight line, this means we have a **linear equation**, and we can use: **y = mx + b** where **y** is the vertical axis value, **x** is the horizontal axis value, **m** is the slope of the line, and **b** is the y-intercept.

Computer programs and calculators can perform a **linear regression** analysis by plotting the "best fit" line through the data and then writing the slope-intercept equation. The **correlation coefficient** (with the symbol "**r**") is a measure of how well the regression line fits with the observed data. A ***perfect*** fit produces a correlation coefficient of either +1.000 (positive slope) or -1.000 (negative slope), depending on if the line slopes up (a positive slope) or down (a negative slope.) The closer the correlation coefficient is to +/-1.000, the better the regression line expresses the data (the better fit for the data.) Note that R^2 is slightly different than r!

Observing the **crystals** of an ordinary substance (such as table salt) using a magnifying glass, one sees many planes at right angles within the solid. This occurs in many common solids, and the regularity we see implies a deeper regularity in the arrangement of atoms or ions in the solid. The atomic nuclei are present in remarkably symmetrical arrays that continue for millions of units in three dimensions. Substances having a regular arrangement of atom-size particles in the solid are called **crystalline**, and the solid material consists of **crystals**. This lab deals with some of the simpler arrays in which atoms or ions occur in crystals and what these arrays can tell us about such properties as atomic sizes, densities of solids, and the efficiency of packing of particles.

Procedural Notes for the Linear Regression Lab: *Complete the problems using the worksheets at the end*

Each linear regression problem will require one or more **computer generated graphs** that will be stapled to the back of the worksheets. Recommended programs to graph your date include **Microsoft Excel** (**free** for MHCC students; see https://www.mhcc.edu/OfficeInstall/), **Apple Numbers** (free with a Mac computer, https://www.apple.com/numbers/), or **Google Sheets** (https://www.google.com/sheets). ***Note*** that Excel Online (the online version of Excel) and iPad/iPhone/Droid versions of these programs will generally not perform linear regressions, so try to use the "full" computer version instead. Calculators will perform linear regressions, but printing from a calculator might be difficult.

Use a **X-Y scatter plot** when graphing these data sets. **The computer program will analyze the data and perform the linear regression analysis** for you. Each program is different, but generally the user selects the actual data points on the X-Y Scatter plot and either right-clicks or control-clicks on the data to see a new menu…. you wish to "Add a Trendline" and "Display the R^2 value". If an equation appears with an R^2 value, you have performed your linear regression. ***Help*** on performing the linear regression lab can be acquired in the Learning Success Center / AVID Center at MHCC. You can also search YouTube for videos (i.e. search "linear regression Excel 2019" and almost inevitably a helpful video appears.)

Converting R^2 to r is not difficult. Take the square root of R^2 to get r. If the value of the slope is a negative number, then the value of r will also be negative…. watch for this in this lab! Calculators will often give both R^2 and r values when linear regression techniques are applied. Information on making an acceptable graph in this class can be found here: https://mhchem.org/lab

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The Linear Regression Problems:

Problem 1: The Relationship Between Celsius and Fahrenheit

In 1724, the German scientist Gabriel Fahrenheit developed a temperature scale based on phenomenon he thought could be easily repeated in laboratories around the world. For his zero degree point, Fahrenheit chose the coldest mixture of ice, water, and salt that he could produce in his laboratory. For ninety-six degrees, he chose what he believed to be normal body temperature. Fahrenheit wanted a temperature scale that could be divided into twelfths. On this scale, pure water freezes at 32 degrees, and pure water boils at sea level at 212 degrees.

A few years later, in 1742, the Swedish scientist Anders Celsius developed a different temperature scale. This scale used pure water as its standard. Zero degrees was the temperature where pure water froze, and one hundred degrees was the temperature where pure water boiled at sea level. Because Celsius had one hundred degrees between the two reference points on his temperature scale, it was called the *centigrade* scale. Recently this was renamed the Celsius scale in honor of Anders Celsius.

A student measures the following data points in the laboratory using two thermometers:

Temperature (°C)	20.0	40.0	60.0	80.0	100.0
Temperature (°F)	67.6	104.8	141.1	175.0	211.1

1. Construct and print a graph of degrees Fahrenheit (y) as a function of temperature in degrees Celsius (x).
2. Using your calculator, determine the mathematical equation of °F as a function of °C as well as the correlation coefficient, r. Record r to at least four significant figures.
3. Using the actual equation: $°F = 1.8°C + 32$ *and* your experimental equation, convert 29.0 °C to °F. Calculate **percent error** = (difference / actual value) x 100% Comment on discrepancies.

Problem 2: Solubility of Lead(II) Nitrate in Water

The solubility of lead(II) nitrate in water was measured as a function of temperature. The solubility is given in units of grams of lead(II) nitrate per 100 grams of water.

Temperature (°C)	20.0	40.0	60.0	80.0	100.0
Solubility (g / 100 g water)	56.9	74.5	93.4	114.1	131.1

1. Graph and print the data; temperature will be the independent (x) variable.
2. Determine the equation of the best-fit line. Record the equation and correlation coefficient.
3. What is the solubility of lead(II) nitrate at 47.0 °C?

Problem 3: Colorimetry

The colors in the visible spectrum of light are shown by a rainbow. Colored substances absorb segments of the visible spectrum of light. Pink solutions, for example, are pink because they absorb green light and transmit all other colors of the visible spectrum. If light of the particular color absorbed is passed through a sample, the amount of light absorbed will be related to the number of absorbing molecules in the light beam. Dilute solutions absorb little light, concentrated solutions absorb more. Typically the amount of light transmitted through the solution is measured; *transmittance* is inversely proportional to *absorbance*. The following data was obtained for the transmittance of 525 nm light by solutions containing different concentrations of permanganate ion.

Concentration (mg/100 mL)	1.00	2.00	3.00	4.00
Transmittance *(unitless)*	0.418	0.149	0.058	0.0260

1. **Convert the Transmittance values to Absorbance** using the following equation: **A = log (1/T)**, where A = Absorbance and T = Transmittance. **Use 3 sig figs for your absorbance values**.
2. Graph and print the Absorbance (y) versus Concentration (x) data. Perform a linear regression analysis. Record the equation and the correlation coefficient.
3. Predict the absorbance of 2.50 mg permanganate ion / 100 mL solution.

Problem 4: Kinetics

The branch of chemistry that studies the rate or speed of reactions is called *kinetics*. One must often plot concentration versus time data in a variety of mathematical formats to find a linear relationship; this assists in finding the *order of reaction*. We shall explore this topic more in CH 222. The following data was collected at 25.6 °C while measuring the disappearance of NH_3:

Concentration [NH_3] (mol/L)	$8.00 * 10^{-7}$	$6.75 * 10^{-7}$	$5.84 * 10^{-7}$	$5.15 * 10^{-7}$
Time (h)	0	25.0	50.0	75.0

1. **Prepare a graph of ln [NH_3] versus time** (time is the x-axis). "ln" stands for natural logarithm which can be calculated easily on your calculator (for example, the value of $8.00 * 10^{-7}$ is -14.039.) Perform a linear regression analysis on the ln [NH_3] versus time data and find the equation and the correlation coefficient. **Use at least 4 sig figs for your absorbance values**.
2. **Prepare a graph of 1 / [NH_3] versus time** (for example, $1 / 8.00 * 10^{-7}$ is $1.25 * 10^{6}$. ***Note:*** You may have to enter the data as "1.25E6" to make the program understand your values.) Time will be the x-axis. Perform a linear regression analysis and find the correlation coefficient and the values for the slope and the y-intercept.
3. **Which graph gives a *better* linear regression?** Why? *Hint:* look for the better correlation coefficient.
4. Plots of ln [NH_3] versus time that are linear are called *first order reactions* while graphs of 1 / [NH_3] versus time that are linear are called *second order reactions*. **What order of reaction** does the decomposition of NH_3 follow? *Hint:* the better linear regression will determine the order of the reaction!

Procedural Notes for the Crystal Structures of Solids Lab: Complete the handouts found at the end of this lab and turn it in (with all relevant work displayed on adjacent pages) to your instructor. Help on completing the "Solids" questions can be acquired in the Learning Success Center / AVID Center at MHCC.

Many crystals are unbelievably complex, and we will limit ourselves to the simplest crystals that have cubic structures. Cubic structures imply 90° angles and sides of equal length (hence, a cube.) We will also limit ourselves to the study of only one kind of system (namely metal elements), yet they will exhibit many of the interesting properties of more complicated structures.

The Simple Cubic (SC) Crystal

The simple cubic unit cell is a cube with an **edge length**, $\mathbf{d_0}$, equal to the distance from the center of one atom to the center of the next (see Figure One). The volume of the cube is equal to $(d_0)^3$, expressed as

$$\mathbf{V = (d_0)^3}$$

and is very small since d0 is on the order of 0.5 nm. Using x-ray diffraction we can measure the value of d0 easily to four significant figures. The number of atoms in a simple cubic unit cell is equal to one, for only 1/8 of each corner atom is actually inside the cell.

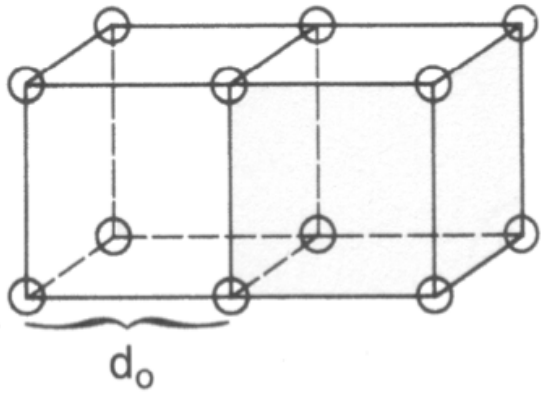


Figure One: *The Simple Cubic Crystal*

Each atom in the simple cubic unit cell is actually connected to six other atoms in the cubic lattice; hence, we say that the **coordination number** of the atoms in this structure is equal to six.

Many diagrams displaying the simple cubic unit cell show a gap between adjoining atoms. **In an actual crystal, we consider that the atoms that are closest are touching**. It is on this assumption that we determine **atomic radii, r**. In the SC crystal, if we know d_0, we can find the radius r of the atoms, since one side contains 2 atomic radii, or

$$\mathbf{d_0 = 2r}$$

for simple cubic crystals. Knowing the radius, we can calculate d0, and then we can calculate the volume of the unit cell. Knowing that one atom occupies the simple cubic cell, we can calculate the mass of the unit cell (using the molar mass and Avogadro's number), and from this we can determine the density using the volume of the cell.

Essentially no elements crystallize in the simple cubic structure, however, due to the inefficiency of the packing. The atoms in the simple cubic crystal are farther apart then they need to be, and inspection of the SC lattice will reveal a large hole in the center of the unit cell. Only about 52% of the cell volume is occupied by atoms, and more "empty space" means less stabilization for the crystal structure.

The Body Centered Cubic (BCC) Crystal

In a **body centered cubic crystal**, the unit cell still contains the corner atoms present in the SC structure, but the center of the cell now contains an additional atom. This means that every BCC crystal structure holds **two net atoms** (eight atoms are $^1/_8$ within the cell, and one whole atom within the center of the cell for two net atoms).

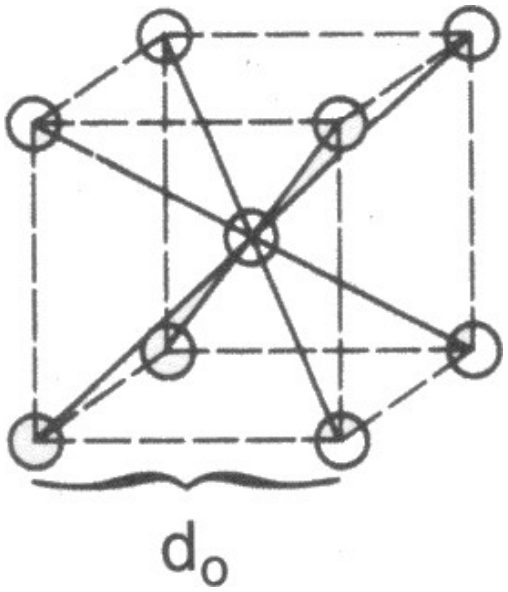


Figure Two: *Body Centered Cubic Crystal*

The edge length, d_0, can be determined using simple geometry from the **cube diagonal** (see Figure Two). The cube diagonal reaches across the cube, from an atom in the lower left front to an atom in the upper right back, or from any other appropriate combination. Geometry dictates the following relationship between the cube body diagonal and the edge length, d_0:

$$\text{cube diagonal} = \sqrt{3} \cdot d_0$$

The cube diagonal encompasses 4 radii lengths, and d_0 can be expressed in terms of the radius of the atom:

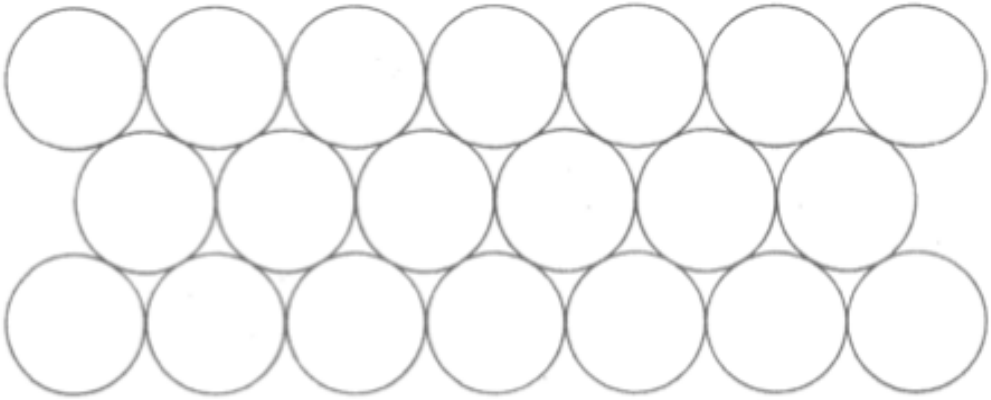
$$d_0 = \frac{4r}{\sqrt{3}}$$

The quantity d_0 can be used to find the volume of the cube; this is important for BCC cubic systems.

In a BCC lattice, each atom touches eight other atoms, and the **coordination number** is eight. The BCC lattice is much more stable than the SC structure, in part due to the higher coordination number. Many metals at room temperature display the BCC lattice, including sodium, chromium, tungsten and iron. Note that there are two atoms per unit cell in the BCC crystal. **BCC crystals are more efficient than SC crystals**, occupying approximately 68% of the total available volume.

Close Packed Structures

Although many elements prefer the BCC crystal arrangement, still more prefer structures in which the atoms are **close packed**. In close packed structures there are layers of atoms in which each atom is in contact with six others, as in the sketch below:



This is the way in which billiard balls lie in a rack or the honeycomb cells are arranged in a bees' nest. It is the most efficient way one can pack spheres, with about 74% of the volume in a close packed structure filled with atoms.

There is more than one way whereby close packed crystal structures can be stacked. One of the stacking methods is cubic and is called the **Face Centered Cubic (FCC)**. The other is called **Hexagonal Close-Packing**. We shall look at both close packed structures.

The Face Centered Cubic (FCC) Crystal

In the face centered cubic crystal unit cell there are atoms in each corner of the cell (as in the SC cell discussed earlier) and there is another atom at the center of each of the six faces. This means that FCC cubic systems consist of **four net atoms** per unit cell (eight atoms are $^1/_8$ within the cell, and six faces hold an atom which is $^1/_2$ within the cell for four net atoms). See Figure Three.

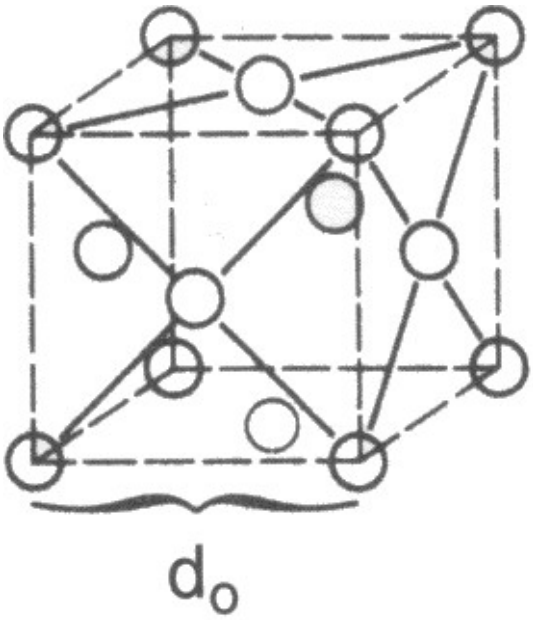


Figure Three: *Face Centered Cubic Crystal*

The edge length d_0 can be determined in an FCC crystal from the **face diagonal** which is defined as the distance across one face of the cube. Using geometry, we can find the edge length from the face diagonal using the following equation:

$$\text{face diagonal} = \sqrt{2} \cdot d_0$$

The face diagonal encompasses 4 radii lengths, and d_0 can be expressed in terms of the radius r:

$$d_0 = \frac{4\text{r}}{\sqrt{2}}$$

This expression can be used to find the volume of the cube; hence, this relationship is important for FCC cubic systems. The **coordination number** in an FCC lattice is 12, implying that FCC lattices are quite stable.

The close-packed layers of atoms in the FCC lattice are not parallel to the unit cell faces, but rather are perpendicular to the cell diagonal. If you look down the cell diagonal, you see six atoms in a close-packed triangle in the layer immediately behind the corner atom, and another layer of close-packed atoms below that, followed by another corner atom. The layers are indeed closely packed, and as one goes down the diagonal of this and succeeding cells, the layers repeat their positions in the order ABCABC…. This implies that atoms in every fourth layer lie below one another (see Figure Four (b)).

Hexagonal Close-Packing

There is another way to stack the layers as in the FCC lattice, above. The first and second layers will always be in the same relative positions, but the third layer could be below the first one if it were shifted properly. This results in a **close-packed structure** in which the order of the layers is ABABAB… (see Figure Four (a))

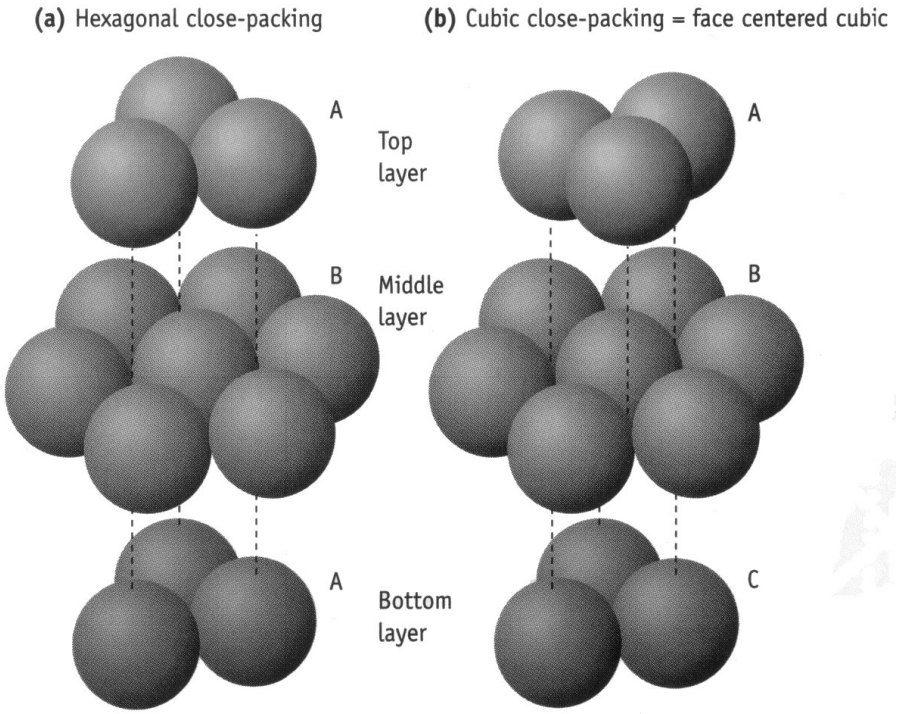


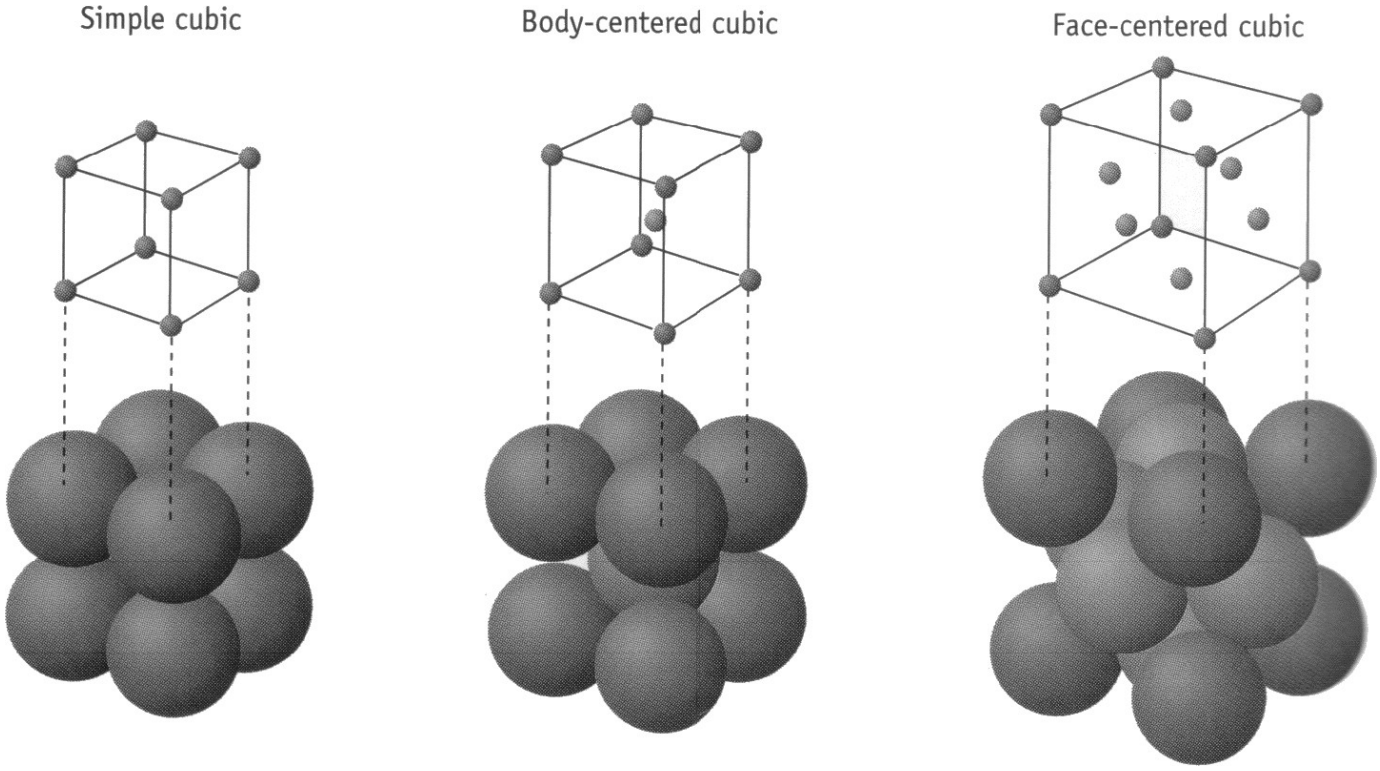
Figure Four: *Hexagonal Close Packing (left) and Cubic Close Packing (right)*

The crystal obtained from this arrangement of layers is not cubic but **hexagonal**. It is another common structure for metals. Cadmium, zinc and manganese have this structure. As you might expect, the stability of this structure is very similar to that of FCC crystals. We find that simply changing the temperature often converts a metal from one form to another. Calcium, for example, is FCC at room temperature, but if heated to 450 °C it converts to close-packed hexagonal.

In CH 222 (and CH 223), we will consider "hexagonal close-packing" structures to be identical to FCC lattices, but technically there are many differences between the two systems.

Summary of Crystal Lattice Types

Figure Five shows the three main cubic unit crystal types that we will explore in this lab. **Figure Six** show a helpful methodology to solve problems like these in this lab.



Lattice Type	**Simple Cubic**	**Body Centered Cubic**	**Face Centered Cubic**
# net atoms per cell	1	2	4
d_0 (edge) in relation to r	$d_0 = 2r$	$d_0 = \frac{4r}{\sqrt{3}}$	$d_0 = \frac{4r}{\sqrt{2}}$

Figure Five: *Summary of the Three Cubic Unit Cell Types*

conversion *V = edge³* *density* *molar mass (g/mol)* *Avogadro (6.022 x 10^{23})*

radius ↔ edge ↔ volume ↔ mass (g) ↔ moles ↔ atoms / molecules

1 pm = 10^{-12} m / 1 Å = 10^{-10} m / 1 cm = 10^{-2} m *4 atoms = 1 fcc cell, etc.*

Figure Six: *Helpful Conversion Methodology*

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Worksheet: Linear Regression & The Crystal Structures of Solids *Name:*

All final answers must be provided on this worksheet. **Include computer generated graphs** (from Excel or a similar program) **along with any necessary calculations** needed for the lab in your submission. Values of r should be recorded to three or more significant figures. **This page *will* be placed at the front of your lab, with your first and last name included, to prevent a point penalty.**

Linear Regression:

- **Problem 1**: ***The Relationship Between °C and °F*** - *see page lb-6-3 for data and questions*

Linear Regression equation: **y =** _____

r = _____ *Percent Error:* _____

- **Problem 2**: ***Solubility of Lead(II) Nitrate in Water*** - *see page* Ib-6-3 *for data and questions*

Linear Regression equation: **y =** _____

r = _____ *Solubility of lead(II) nitrate at 47.0 °C:* _____

- **Problem 3**: ***Colorimetry*** - *see page* Ib-6-4 *for data and questions*

Linear Regression equation: **y =** _____ **r =** _____

Absorbance of 2.50 mg permanganate in 100 mL solution: _____

Linear Regression: *Continued*

- **<u>Problem 4</u>:** ***Kinetics*** - *see page* Ib-6-4 *for data and questions*

Linear Regression (ln [NH_3] vs. time) equation: **y =** _____ **r =** _____

Linear Regression (1/[NH_3] vs. time) equation: **y =** _____ **r =** _____

Which regression gives a better linear regression? Why?

Does this data behave as a first order reaction or a second order reaction?

- **<u>Problem 5 *(Use the data from the video)*</u>:** Experimentally determine the density of an unknown metal solid to at least three significant figures using the displacement method. Report and use the data from the lab video.

Relevant calculations and data:

The Crystal Structures of Solids:

- **Problem 6:** What element forms a face centered cubic cell, has a density of 8.92 g/cm^3, and a radius of 128 pm?

Element = _____ *Show relevant work below*

The Crystal Structures of Solids: *Continued*

- **Problem 7:** Chromium forms a body centered cubic crystal. If the length of an edge is 2.884 angstroms, calculate the **density** (g/cm^3) and the **radius** of a chromium atom in angstroms.

density (g/cm^3) = _____ **radius (Å) =** _____

Show relevant work below.

The Crystal Structures of Solids: *Continued*

- **Problem 8:** Sodium (radius = 186 pm) forms a body centered cubic crystal. Calculate the **density** (g/cm^3) of sodium metal. **Propose a simple experiment to confirm your calculated density of sodium** in the lab.

density (g/cm^3) = _____

Show relevant work below.

Proposed simple experiment:

The Crystal Structures of Solids: *Continued*

- **Problem 9:** Aluminum crystallizes in a face centered cubic unit cell. In addition, aluminum has an atomic radius of 143 pm. What is the density of aluminum?

density (g/cm^3) = _____

Show relevant work below.