

LAB II CRYSTAL STRUCTURE

Study Questions:

1. What properties of a strongly bonded covalent solid like diamond can be attributed to its bond type?
 2. Explain why covalent bonds are directional but ionic bonds are not.
 3. Show the electron notation of Cu, Cu^{+1} , and Cu^{+2} .
 4. Explain why a simple ionic crystal like CsCl cannot crystallize into a BCC structure.
 5. Graphite is very anisotropic; that is, its properties are dependent on crystallographic direction. Given a cross-section of graphite, try to explain why the electrical conductivity of graphite is 100 times greater in the horizontal direction than in the vertical.
 6. Consider an FCC unit cell with the lattice parameter 'a'. Calculate the diameter of the atoms making up this unit cell.
 7. For a cubic crystal system, how many $\langle 110 \rangle$ directions are contained in the (111) plane?
 8. For a cubic crystal system, label the following: [100], (112), [123], and (123).
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Lab:

I. Crystal Structure

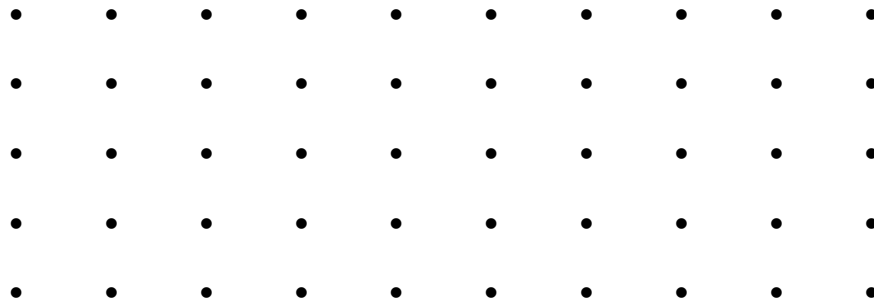
A *lattice* is a regular array of points repeated through space. The *Bravais lattices* are the 14 different lattices possible in 3-dimensional space. A crystal structure is a three dimensional arrangement of atoms or groups of atoms in space that can follow any of the 14 Bravais lattices. A primary unit cell is the smallest repeating unit of a crystal structure. Unit cells are parallelograms in two dimensions and parallelepipeds in three dimensions.

The size and shape of a unit cell is described, in three dimensions, by the lengths of the three edges (a, b, and c) and the angles between the edges (α , β , and γ). These quantities are referred to as the *lattice parameters* of the unit cell. For a cubic unit cell, $a=b=c$ and $\alpha=\beta=\gamma=90^\circ$. Note that although different materials may have the same unit cell and crystal structure, they will not have the same lattice parameters.

I.1 What would explain the difference in lattice parameters between materials with the same crystal structure (e.g., BCC)?

The selection of a unit cell is not unique; the corners of a unit cell may actually be any where within the space of the lattice, provided that repeated translations of this chosen cell will fill all of the space of the lattice. Conventional practice is to choose the smallest, simplest, most expressive and symmetric unit cell for the lattice.

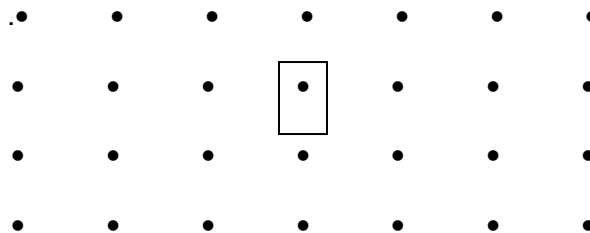
I.2 Here is a two-dimensional grid of dots. Draw 3 unique unit cells on this grid, with cell corners on dots, labeling the unit cells as A, B, and C, respectively. Next, determine each cell's lattice parameters a , b , and α (here, the smallest angle between any a and b). Finally, give the number of dots in each cell (assuming that any lines intersect the exact middle of dots, so a dot on a line will *not* be a whole dot!).



The horizontal distance between adjacent dots is ' x ' and the vertical distance between adjacent dots is ' y '. Express ' a ', ' b ', and ' α ' (if necessary) in terms of these.

unit cell	a	b	α	# dots in unit cell
A				
B				
C				

I.3 Other than not having its corners on dots, would the following cell be a valid unit cell? If not, why not?



II. Two - Dimensional Packing

Use pennies to represent a two dimensional array of atoms. There are two basic configurations: square packing and close packing.

First, arrange the pennies into square packing and answer the following questions:

II.1 What is the coordination number (number of nearest neighbors or pennies touching) of one penny in this arrangement? _____

II.2 Draw the simplest unit cell (must be more than one penny!) for this packing configuration and indicate all close packed directions.

II.3 What is its value for α ? _____

II.4 Give an expression for the unit cell lattice parameter 'a' in terms of penny radius 'r'.

a= _____

II.5 Find the packing fraction (i.e., packing efficiency) for your unit cell: _____
(defined as area of the atoms divided by the area of the unit cell)

Now arrange the pennies into close packing and answer the following questions:

II.6 What is the coordination number (number of nearest neighbors or pennies touching) of one penny in this arrangement? _____

II.2 Draw the simplest unit cell (must be more than one penny!) for this packing configuration and indicate all close packed directions.

II.8 What is its value for α ? _____

II.9 Give an expression for the unit cell lattice parameter 'a' in terms of penny radius 'r'.

a= _____

II.10 Find the packing fraction (i.e., packing efficiency) for your unit cell: _____
(defined as area of the atoms divided by the area of the unit cell)

III. Three - Dimensional Packing

The four most basic crystal structures are:

- Simple cubic (SC)
- Body centered cubic (BCC)
- Face centered cubic (FCC)
- Hexagonal close packed (HCP)

You should develop a complete understanding of the geometry and atomic arrangement of each of these structures. Make a sketch of each of these structures below.

III.1 Simple Cubic

III.2 Body Centered Cubic

III.3 Face Centered Cubic

III.4 Hexagonal Close Packed

Now *construct* each of these four crystal structures using Styrofoam balls and toothpicks. You should strive to completely understand the atomic packing and geometry of each of these structures. Begin by creating the individual layers, and then stack each layer together to compose the structure. To test your understanding you should discuss the similarities and differences between the structures in your team. Be sure that you can completely visualize each structure.

III.5 For each structure determine the following:

Structure	atoms/cell	coordination #	APF	$a = f(r)$
SC				
BCC				
FCC				
HCP				

Which two structures show the greatest similarities? _____ and _____

Consider the BCC and FCC structures you have built:

III.6 Which crystal has the largest interstitial site? _____

III.7 Does the size of the interstitial sites in each crystal type correlate with APF? (i.e., does a higher APF mean smaller interstitial sites?) _____

III.8 There are 2 different types of interstitial sites for BCC crystals. How many of each type are there? Indicate in a sketch where each is.

III.9 There are 2 different types of interstitial sites for FCC crystals. How many of each type are there? Indicate in a sketch where each is.

III.10 If material properties (tensile strength, conductivity, etc) are a function of crystal structure, will the measured properties of some materials vary with crystal orientation? How can you explain this?

IV. Ionic Structure

Although we have been examining single element crystal structures, the same principles apply to ionic structures composed of two or more elements. In this case we find the bonding to be predominately ionic, rather than metallic or covalent, which has several implications.

In your textbook, there is a discussion of coordination numbers and geometries that are dependent on the cation-anion radius ratio in the ionic compound: r_c/r_a . Stable ceramic crystal structures form when anions that surround a cation are all in direct contact with the cation, and the coordination of that cation is related to the cation-anion radius ratio.

IV.1 Given an ionic radius for Na^+ ion = 0.95\AA and for Cl^- = 1.81\AA , what is the cation to anion radius ratio for NaCl?

$$r_c/r_a =$$

IV.2 Referring to the range of radius ratios to coordination numbers (in Callister), what is the coordination number of the Na^+ ions in the NaCl structure?

$$C\# =$$

IV.3 Make a three dimensional sketch of the NaCl structure below, indicating which are the Na^+ and Cl^- ions. The ions should be roughly in scale relative to one another: that is, they should *not* be drawn having the same size.

IV.4 How many Na^+ ions are present within the cell? _____ How many Cl^- ions are present? _____ Is there charge neutrality within the cell? _____

IV.5 How might you explain the brittle nature of ceramics? Consider that ceramic materials are composed of two or more ionic species, while metals are not. They both form similar crystal structures, why is one so much more brittle than the other?