Lab 2: Structure of Crystalline Solids

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EE 145L
Section: Tuesday 9:00-11:00am

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1 Abstract

The purpose of this lab is to use the solid state modelling kits to help visualize coordination numbers and lattice structures. There are also a set of exercises that give practice with miller indices and characterizing lattice structures. The models were all built and photographed except for the last three due to time constraints, and the exercises were performed and presented.

2 Introduction

When atoms form solids, through one of the bonding mechanisms e.g. ionic or covalent, they can form either amorphous solids, crystalline solids or polycrystalline solids. Amorphous solids have no discernible structure. Polycrystalline solids are made of many misaligned crystalline substructures. Crystalline structures are made of discernible repeating patterns, and are the subject of this lab.

To define a crystal structure, two things must first be defined: The lattice and the basis. The lattice is a set of points dispersed in space where any point can be reached from any other point by an integer combination of N predefined vectors for an N-dimensional space. The lattices dealt with in this lab are 'simple cubic', 'body-centered cubic' and 'face-centered cubic'. A basis is a basic configuration of atoms that is placed at each lattice point to fully construct the crystal.

The purposes of this lab are to: work with the atomic modelling kits to visualize different lattices and crystal structures, practice drawing planes and directions using miller indices, and characterize basic cubic, body-centered cubic and face-centered cubic lattices.

3 Materials and Methods

Materials:
- Solid state atomic structure modelling kit

Methods:
To construct each model, first the guide-card specified in the directions was retrieved from the bag and placed on the correct base-plate. Metal rods were placed in the holes according to the modelling-kit instructions. The structure was then constructed layer by layer using the specified colored spheres from the modelling kit, and according to the instructions.

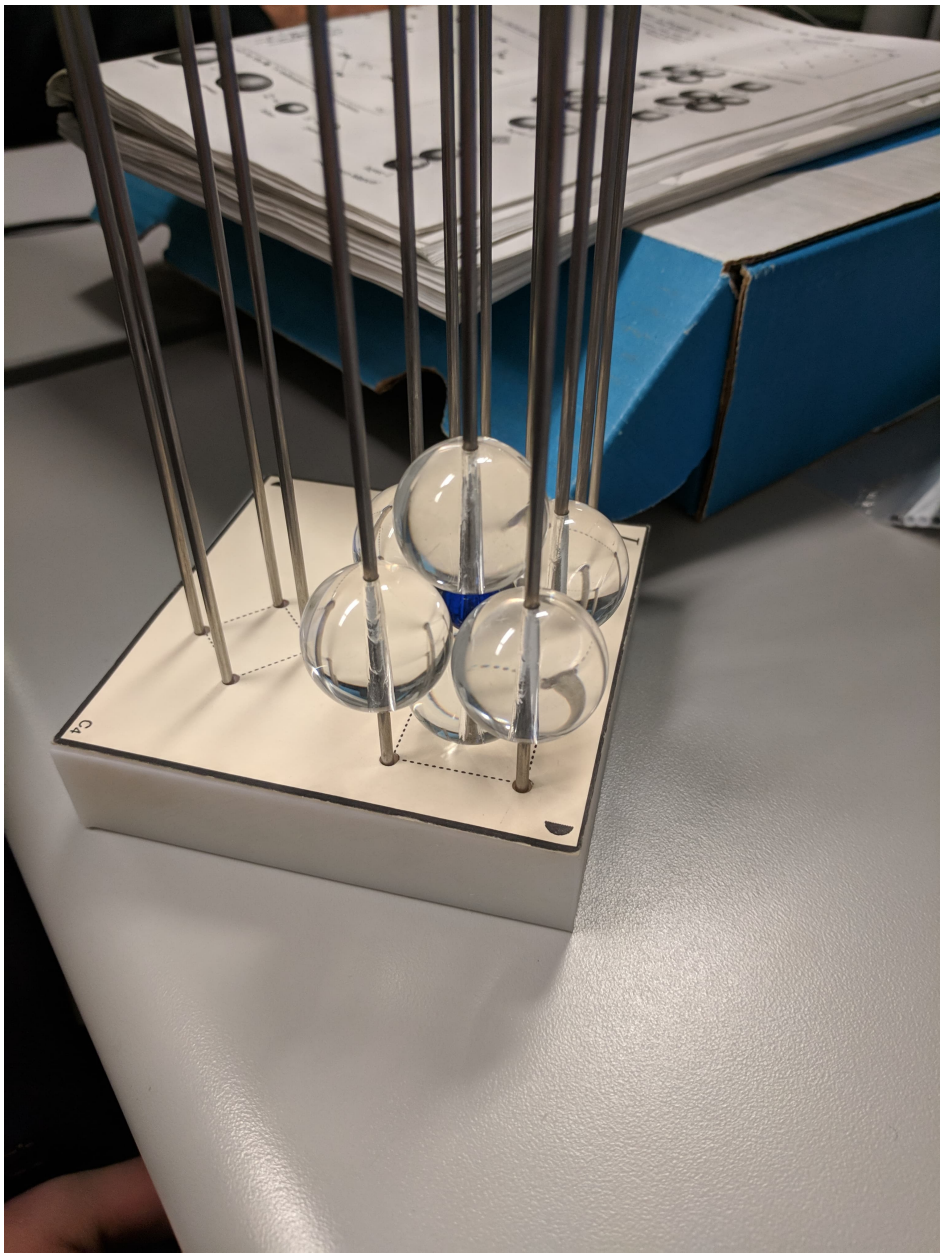


Figure 1: Compound with CN6 from pg 93

4 Results and Analysis

Coordination Number Questions:

1. Which set of structures represent compounds and why?

A compound is defined as a chemical consisting of more than one type of chemically bonded element. Therefore, the structures shown in Figure 1, Figure 2 and Figure 3 represent compounds because they are structures consisting of more than one type of atom. This is assuming that the different colored spheres represent different elemental atoms.

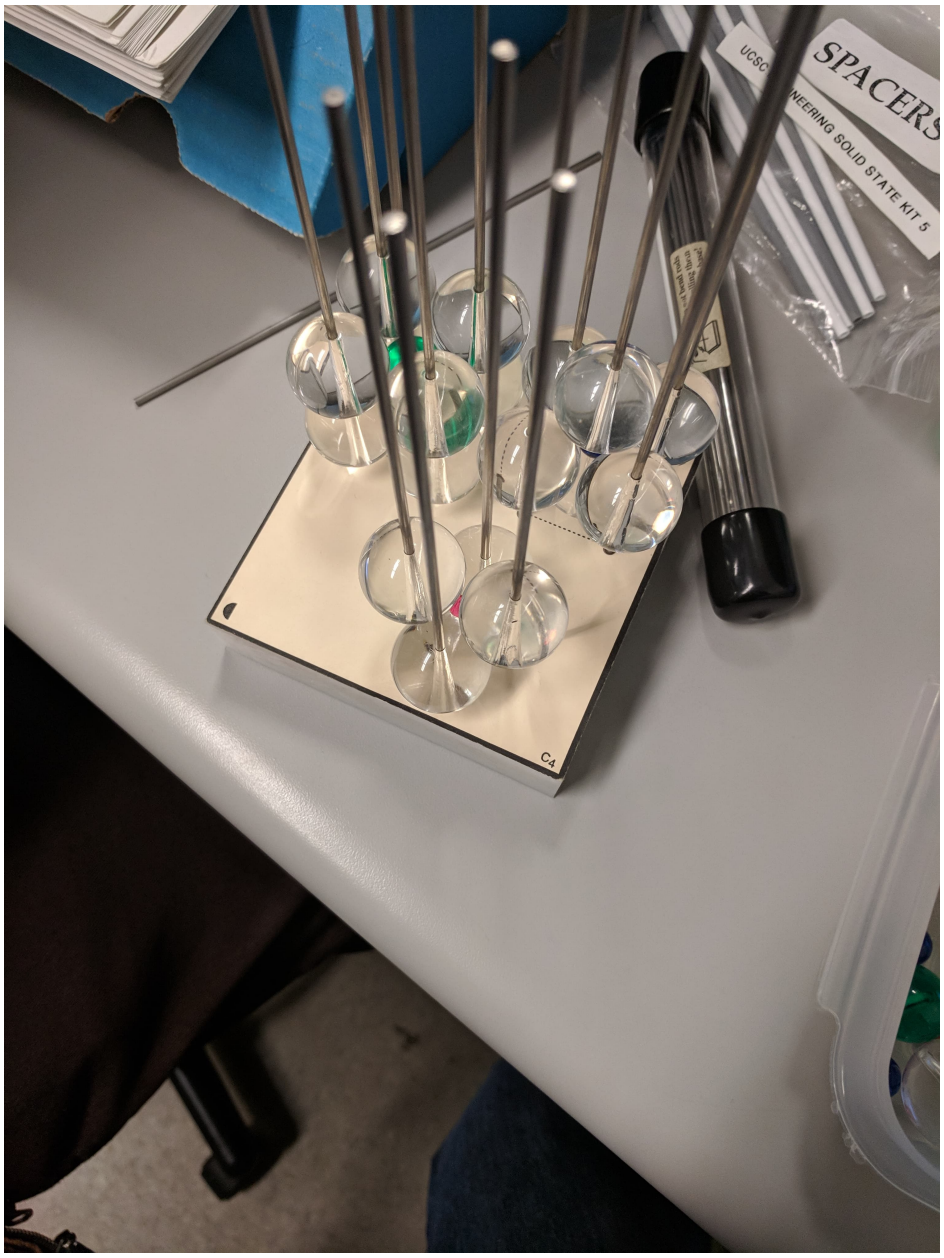


Figure 2: Compound with CN4 from pg 93

2. What is the maximum number of nearest neighbors you can have for a structure with a single element?
The maximum coordination number for a structure of a singe element is 12. This is exemplified by the hexagonal close-packed and face-centered cubic structures. There are no single-element structures with a coordination number of more than 12.

3. How many nearest neighbors do an octahedral and tetrahedral atom have?
Examples of octahedral and tetrahedral structures are shown in Figure 1 and Figure 5 respectively. Therefore, the coordination numbers of octahedral and tetrahedral atomic structures are 6 and 4 respectively.

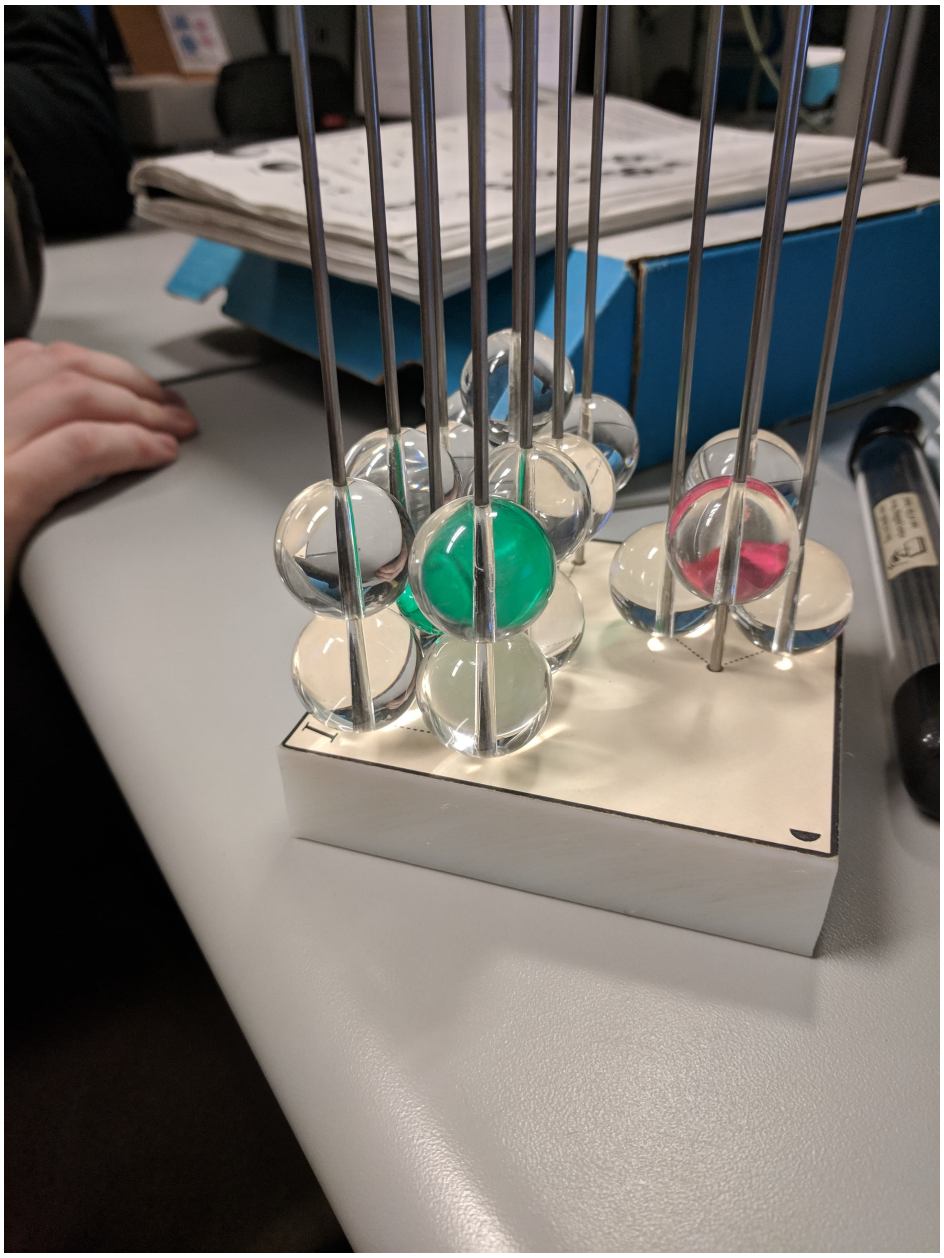


Figure 3: Compound with CN8 from pg 93

Exercise 1:
My solution to Exercise 1 is shown in Figure 6. Note that for part c, the [211] direction is difficult to see, and is near the origin when viewed from this perspective.
Exercise 2:
My solution to Exercise 2 is shown in Figure 7. Note that in part c, the (321) plane is difficult to see as it is also near the origin. Also, two the dots that mark the plane's intersections with the the major axes overlap with those of the other two planes, making it even more difficult to see.
Characterization of Cubic Lattices:
My solution for the Cubic lattices questions are shown in Figure 8. For the 7th and 8th questions,

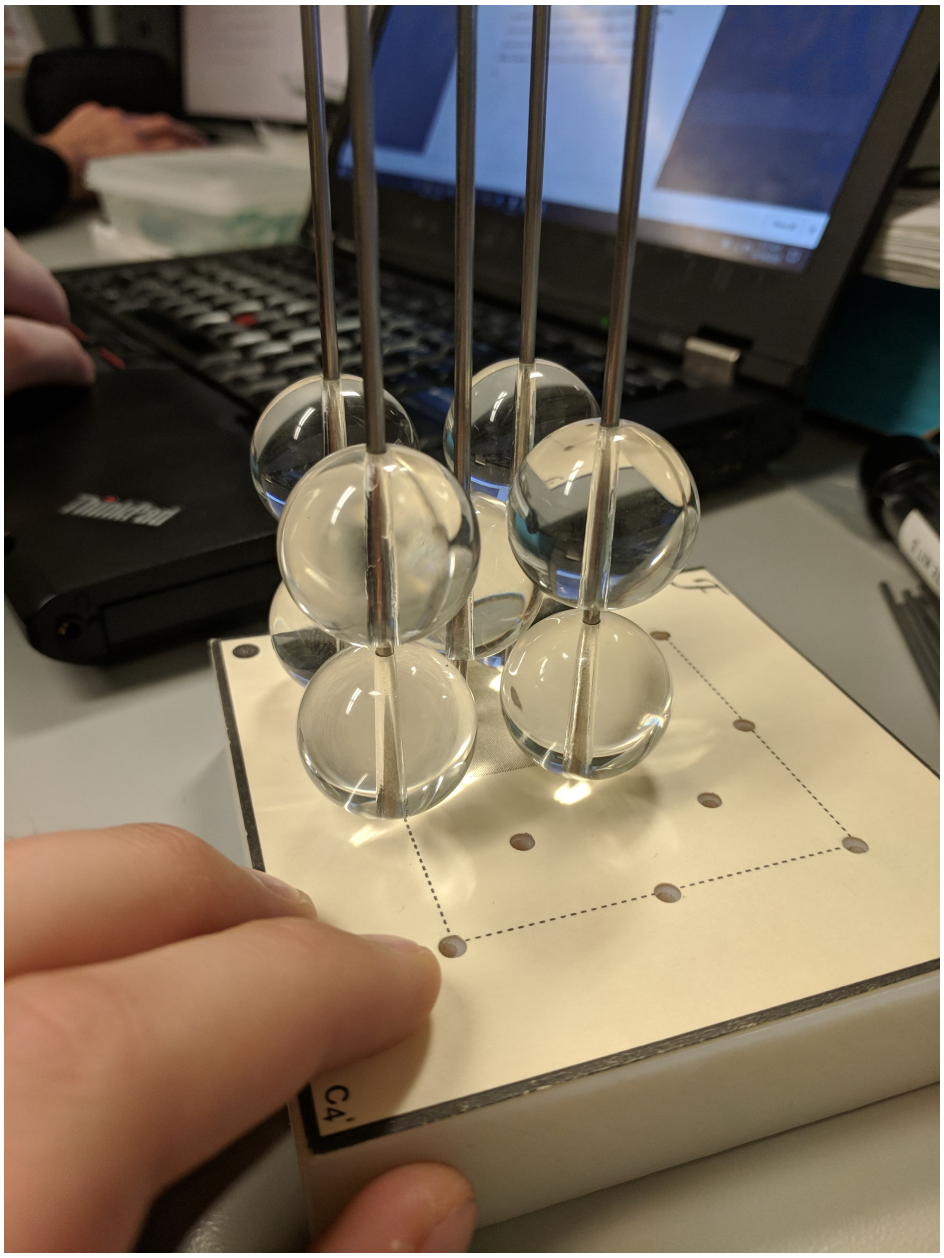


Figure 4: Single atom structure with CN8 from pg 100

I assumed that you start with the unit cell occupied by the portions of atoms that fit within the unit cell, and that you then say which of those atom-portions intersect with the direction/plane and give the sum of their portions. For question 9, I gave the answer in terms of planar groups to signify that all of the planes of that group have equal atom density.

5 Conclusions

During this lab, we practiced using miller indices to identify planes and directions. We used the solid state modelling kit to visualize atomic structures and coordination numbers. We also used the

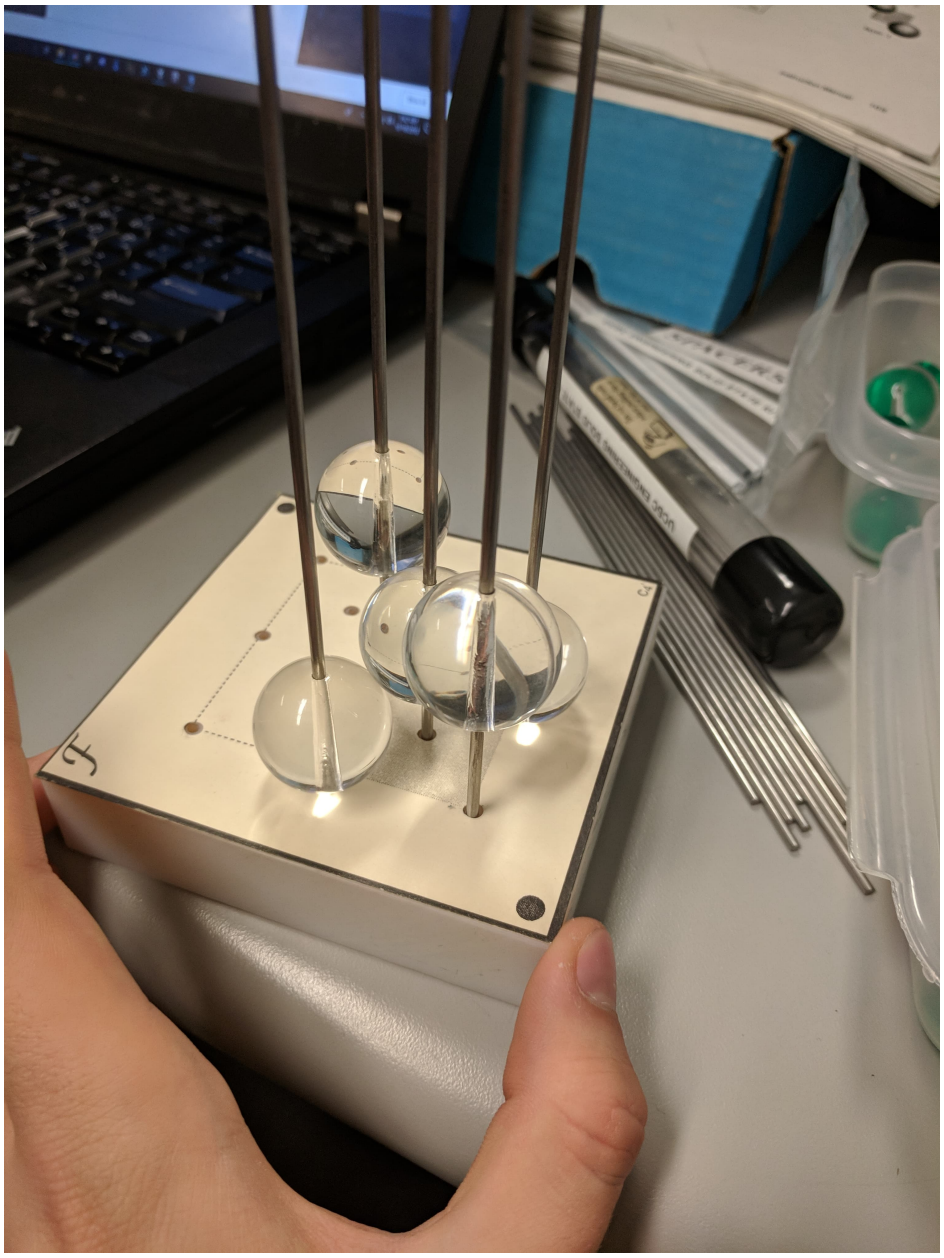


Figure 5: Single atom structure with CN8 from pg 103

modelling kits to characterize the three cubic lattice structures. All of the exercises were performed to the best of my ability. All of the models were created and photographed except for the SC, BCC and FCC models due to time constraints. During this lab I realized that the number of 'lattice points in a unit cell' means the number of **unique** lattice points one can place on the unit cell and still fully define the lattice via translation and replication of the unit cell.

Lab Section 2a

Crystal Directions

***Exercise* I**

Draw the following directions in the cubic unit cells shown below:

(A) [100] [010] [001] (all in the same unit cell)

(B) [111] [$1\bar{1}1$] [$\bar{1}\bar{1}1$] (all in the same unit cell)

(C) [121] [112] [211] (all in the same unit cell)

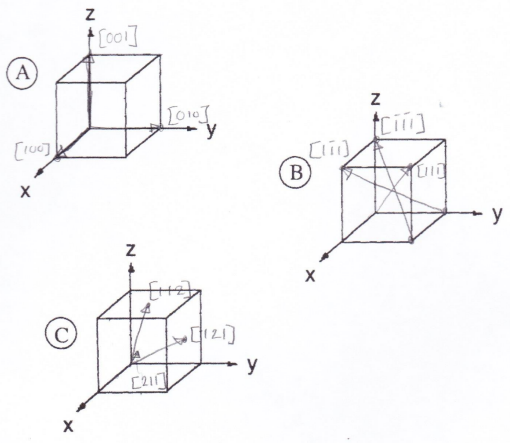


Figure 6: Exercise 1 Solution

Lab Section 2b

Crystal Planes

Exercise 2

Draw the following planes in the cubic unit cells shown below:

(A) (100) (010) (001)

(B) (110) (101) (011)

(C) (121) (211) (321)

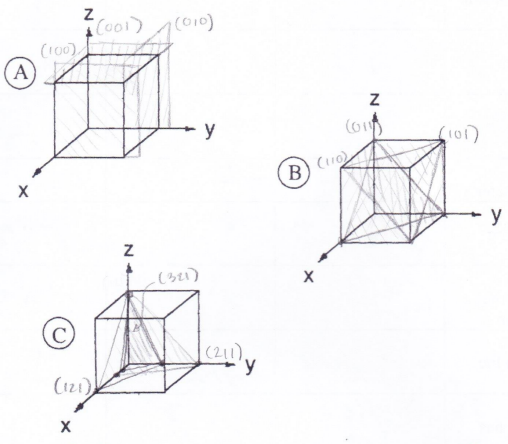


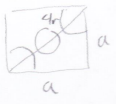
Figure 7: Exercise 2 Solution

Lab Section 3

Crystal Systems and Bravais Lattices:

Build the models for simple cubic (SC) pg. 9, Body Centered Cubic pg., 18, and Face-Centered Cubic pg.27 and answer questions in the table below.

	Simple Cubic	Body Centered Cubic	Face Centered Cubic
# of atoms in the unit cell?	1	2	4
# of lattice points in the unit cell?	1	2	4
# of atoms per basis?	1	1	1
Coordination Number?	6	8	12
Lattice Parameter a?	$2r$	$\frac{4\sqrt{3}}{3}r$	$2\sqrt{2}r$
Atomic Packing Factor?	52%	68%	74%
# of atoms in the [111] direction	1/4	1 1/4	1/4
# of atoms on the (110) plane?	1/2	1/2	1
Which plane has the highest atom density?	{100}	{110}	{110}



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

$16r^2 = 2a^2$

$8r^2 = a^2$

$a = 2\sqrt{2}r$

$4 \cdot \frac{4\pi}{3} r^3$

$(2\sqrt{2}r)^3$

$\frac{4\pi}{3}$

$8\sqrt{2}^3$

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Figure 8: Cubic Lattices Characterization Table