ENGR270 Lab 3

Making Cubic Crystal Structures with Styrofoam Balls

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Abstract

This experiment was about coming up with an experimental value for the atomic packing factor of FCC, BCC, and SC structures of cubic crystals. The experiment utilized Styrofoam balls and toothpicks to replicate the three geometric structures. The results were fairly close to the theoretical values and within a reasonable error percentage.

Introduction

Atomic packing factor (APF) refers to the volume of atoms contained in a unit cell of a crystal per volume of the unit cell. A unit cell is the smallest volume of repeatable pattern in a crystal. If we assume that the atoms have hard shells and so only come as close as their radius width apart, the APF tells us the percent of a unit cell that is filled with atom (the rest being vacuum).

Equation 0:

APF = volume of atoms per unit cell / volume of unit cell

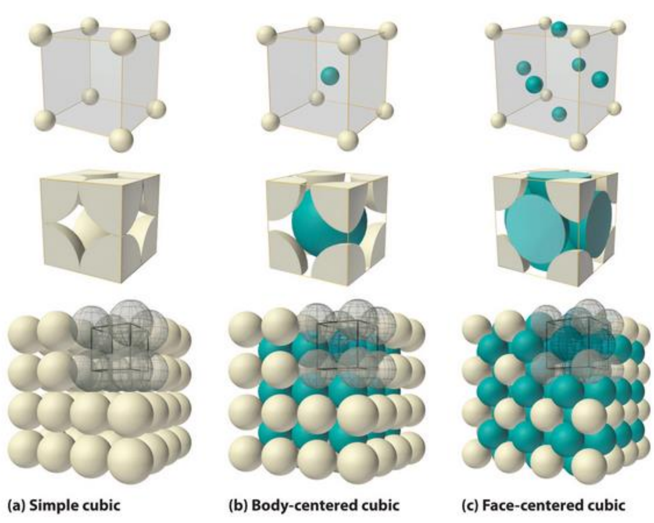

Figure 1 A diagram demonstrating the geometry of SC, BCC, and FCC structures

In order to find the numerator term in Equation 1, we refer to the type of crystal lattice, or the geometry of the atomic structure of the bonds of the atoms in a crystal. There are several different shapes and packing arrangements for unit cells, but in this lab we only examined three: the Simple Cube (SC), Body-Centered Cube (BCC) and Face-Centered Cube (FCC).

The SC unit cell has an atom for every corner of the cell, with the atoms on each side touching each other. The BCC unit cell has an atom for each corner in addition to an atom in the center. An FCC has an atom in each corner of the unit cell and also an atom in the center of each face with no atom in the middle.

The theoretical APF for SC, BCC, and FCC is found in this manner.

Equation 1:

*APF = number of atoms inside unit cell * 4/3 * pi * R^3 / a^3*

a = side length
R = atomic radius

for SC,
number of atoms in each unit cell = 1
a = 2R
for BCC,
number of atoms in unit cell = 2
a = 4R/sqrt(3)
for FCC,
number of atoms in unit cell = 4
a = 4R / sqrt(2)

Thus, plugging in the numbers, the result is that the theoretical APFs for SC, BCC, and FCC are 0.52, 0.68, and 0.74 respectively. These can be reported as percentages.

It was the goal of this lab to prove that the geometry behind the theoretical atomic packing factors is sound within the boundaries of the uncertainty of the experiment.

Methods Used

The materials used in the lab were:

Several Styrofoam balls, at about a 25 mm diameter

Toothpicks

Vernier Calipers

Figure 2 Me, measuring the diameter of the Styrofoam balls

First, I measured all the Styrofoam balls to ascertain their average radius. Then I started creating the unit cell structures by sticking the toothpicks in the balls where the Styrofoam "atoms" were to connect.

My method of connecting the balls was largely to snap the toothpicks in half, poke the dull end into one ball and stick the ball/toothpick combination onto another ball with the sharper end of the toothpick sticking out. This method proved easier for recombination.

Figure 3 My SC cube mid-construction

For the SC structure, it was helpful to start with the first four balls that were to represent the first four corners of the bottom of the cubic unit cell as you can see in Figure 3.

For the BCC, I started with the structure you can see in Figure 4. Then, I added styrofoam balls to the center ball in order to complete the structure. I was able to reposition them when I mistook the angle and was able to come up with a good result. Figure 5 shows what the BCC looked like mid-process.

Figure 5 Attaching the balls together in my BCC model

Figure 4 BCC model halfway finished

For the FCC, I started in the same way as for BCC, except I what I started with became the base as with my contrction of the SC. I expanded outward from there.

Figure 6 FCC in process

Figure 7 FCC in process

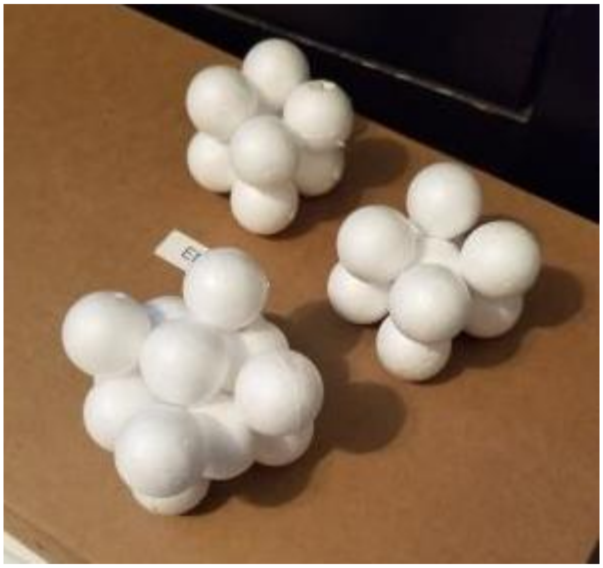

Figure 8 All three finished structures

After finishing construction of all three cubic structures, I measured each of 12 edges with the calipers and calculated the average for each structure. Then, I calculated the edge length for the unit cell with the following formula:

Equation 2:

*Unit cell edge length = edge length – (2*avg radius)*

From Equation 2, I was able to input unit cell edge length in as "a" in Equation 1 to find the APF for each of my constructed Styrofoam cubes.

I was then able to compare the APF I calculated and the theoretical APF.

Results

Unit cell	R_{av} (mm)	δR (mm)	a_{av}(mm)	δa (mm)	Experimental APF_{av}	δAPF	Theoretical APF
SC	12.347	0.096	24.306	0.445	0.549	0.060	0.540
BCC	12.347	0.096	28.881	2.172	0.673	0.227	0.680
FCC	12.347	0.096	35.306	1.457	0.723	0.126	0.740

Table 1: Displays results from calculations as well as standard deviations and uncertainty.

The experimental value for APF I calculated for the SC was 0.549 with an uncertainty of 0.060. For the BCC I calculated an APF of 0.673 with an uncertainty of 0.227 and for the FCC I calculated an APF with 0.723 with an uncertainty of 0.126. The theoretical values for APF were all the same as the Experimental APF values I calculated taking uncertainty into account.

Discussion

The experiment was to determine the legitimacy of the geometric theory of atomic packing. The experiment, though flawed, created results that very closely resembled the theoretical values for APF.

Some errors that may have cropped up to account for the differences in average APF:

The SC was easy enough to "eyeball" given that its angles were all 90 degrees and the set-up was very straightforward. However, there was a lot of guesswork to the BCC. I think that in the future, should I try recreating this experiment, I might try an approach whereby I create a sort of scaffold with the toothpicks instead of the method I used where I guessed at the angles and repositioned them later when they didn’t look quite right. The FCC was especially challenging to keep together and it even fell apart shortly after I finished measuring it. In the future I might want to use some glue once I am sure of the structure.

I believe this experiment does have some merit as it allowed me to more easily visualize the atomic packing structure. Since 3-dimensional software is no substitute for building something with your own hands and seeing a real object with your own eyes, I would recommend other students repeat this experiment in order to stretch their 3-d imaging capabilities.

Acknowledgements

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Citations

https://chem.libretexts.org/Bookshelves/General_Chemistry/Book%3A_Chemistry_(Averill_and_Eldredge)/12%3A_Solids/12.2%3A_The_Arrangement_of_Atoms_in_Crystalline_Solids