Using SolidWorks to improve student's understanding of typical crystal structures

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1. INTRODUCTION

Materials science is a required course in our Mechanical Engineering Program. One important topic which is covered in this course is the crystal structures of crystalline solids [1~4]. The typical crystal structures are body-centered cubic (BCC) crystal structures, face-centered cubic (FCC) crystal structures, and hexagonal closed-packed (HCP). Without a good understanding of these crystal structures, students will have difficulty grasping the concept of unit cell parameters such as side length, atomic packing factor, crystallographic direction, crystallographic plane, tetrahedral site, and octahedral site. The textbook which is used for this course has clear descriptions with clear diagrams of these crystal structures. For example, a unit cell, a reduced sphere-unit cell representation, and an aggregate of many atoms of a faced-centered cubic crystal structure are displayed in Figure 1 and explained in the textbook [1]. However, some students have a hard time developing the spatial thinking skills required to understand typical crystal structures [2~6].

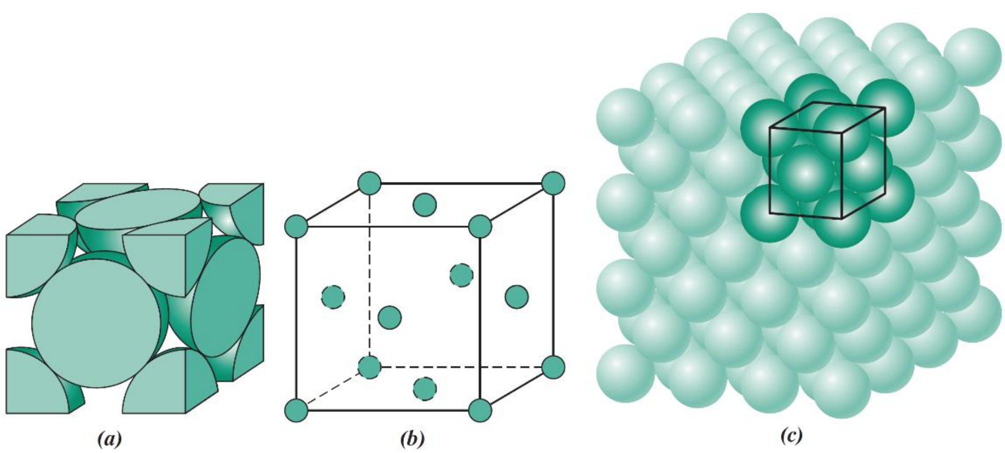


Figure 1 The face-centered cubic crystal structure: a) A hard-sphere unit cell representation, b) A reduced sphere unit cell, and c) An aggregate of many atoms [1]

The materials science course at our school has a physical lab related to this topic. In this lab, ping-pong balls are used to represent atoms, and adhesive is used to connect them together based on the definitions of a given crystal structure. This lab significantly helped students to develop spatial skills and an understanding of typical crystal structures. Based on observations and discussions over the past several years, it was found that some students still had difficulty understanding the basic concepts of typical crystal structures. We discovered that there were three issues related to this physical lab. One was that some measurements of the unit cell parameters such as unit cell constant and atomic packing factors had very big relative errors when compared with theoretical values. The second issue was that students only build crystal structure representations with a minimum number of ping-pong balls, could not get a unit cell, or could not repeat the unit cell. The third issue was that they didn't have access to their physical models after the lab session concluded. These physical models were left in the lab and were recycled for future use.

The authors proposed a new approach to reinforce and facilitate students' understanding of typical crystal structures. This approach is to add a virtual SolidWorks lab where the virtual representation of typical crystal structures is created by Solidworks. This paper will present the proposed new approach, its implementation, and class survey based on the data collected.

2. THE PROPOSED NEW APPROACH

In our mechanical engineering program, the materials science course is offered in the junior year. This course has four credits consisting of 3 hours of lecture and two hours of lab. The required textbook is "Materials Science and Engineering: An Introduction" by Dr. William D. Callister. The lecture part of the course covers the fundamental concepts and knowledge of materials science, and the labs are used to demonstrate or physically explain some fundamental concepts discussed during the lectures.

After lectures and a physical lab of typical crystal structures, some students still had some difficulty in better understanding typical crystal structures and had three issues mentioned in the introduction section. We would like to find some solution to help these students.

Many publications address the fact that students will have a much better understanding of a topic if the same topic is presented to students in different ways [7~13]. Multiple exposures of the same topics such as crystal structure were proposed as a new approach. In our mechanical engineering program, students are required to learn how to use SolidWorks to create models and drawings in their freshman year and they continuously use SolidWorks in different courses. By the time students are in their junior year, they will be comfortable using Solidworks to create models. We proposed to add a new virtual SolidWorks lab about typical crystal structures, in which, one-inch radius virtual spheres (SolidWorks part) are used to represent atoms and are assembled per the definitions of typical crystal structures. By using SolidWorks, students can build 3D models to represent these typical crystal structures. They can cut the models to get the unit cells, repeat the unit cells, and view them in different orientations. The measurements of unit parameters based on the SolidWorks models are the same as theoretical values. Since such SolidWorks models are virtual models students can access them at any time and can rotate them in any orientation. Therefore, the new addition of a virtual lab of the typical crystal structures using SolidWorks successfully addresses the three issues mentioned in the introduction.

To help students to have a better understanding of typical crystal structures, we proposed to expose this concept in four different methods: lecturing, virtual representation of typical crystal structures by SolidWorks, physical presentation of typical crystal structures, and homework. This paper will be focused only on the lab portion. Next, we will explain the virtual SolidWorks lab and the physical lab of typical crystal structures.

3. VIRTUAL AND PHYSICAL LABS OF TYPICAL CRYSTAL STRUCTURES OF CRYSTALLINE SOLIDS

The primary purpose of both labs was to provide visualization of typical crystal structures to help students to have a better understanding of the arrangement of atoms. Once the topic of descriptions of typical crystal structures such as BCC, FCC, and HCP structures was covered, the virtual lab of typical crystal structures then was conducted and the physical lab of typical crystal structures is performed after that.

3.1 VIRTUAL LAB OF TYPICAL CRYSTAL STRUCTURES BY SOLIDWORKS

The objectives of the virtual SolidWorks lab of typical crystal structures are to study the atomic arrangements of typical crystal structures by using spheres of one inch in radius as representations of atoms in SolidWorks. By creating the crystal models using SolidWorks parts, students will obtain a tangible grasp of the arrangements of atoms in 3D space and have a better understanding of the similarities, and differences among each of the three BCC, FCC, and HCP crystal structures.

The activities of this virtual lab include the following main items

1) In part mode, create a sphere with a radius of one inch with the center at the origin point, which is used to represent atoms.

2) Study the definitions of BCC, FCC, and HCP structures and the representation of their reduced sphere unit cells provided in the textbook [1]. Use the 3D sketch in the SolidWorks assembly mode to create a lattice for each typical crystal structure which are displayed in Figures 2, 3, and 4. In these figures, the left picture is the lattices of unit cells, where the * point is the center of the atoms (spheres) and the right picture is the reduced sphere unit cells[1].

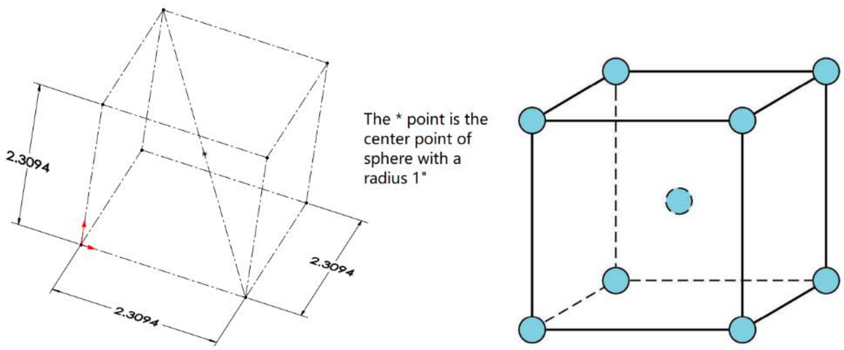


Figure 2 The center points of spheres of the BCC structure

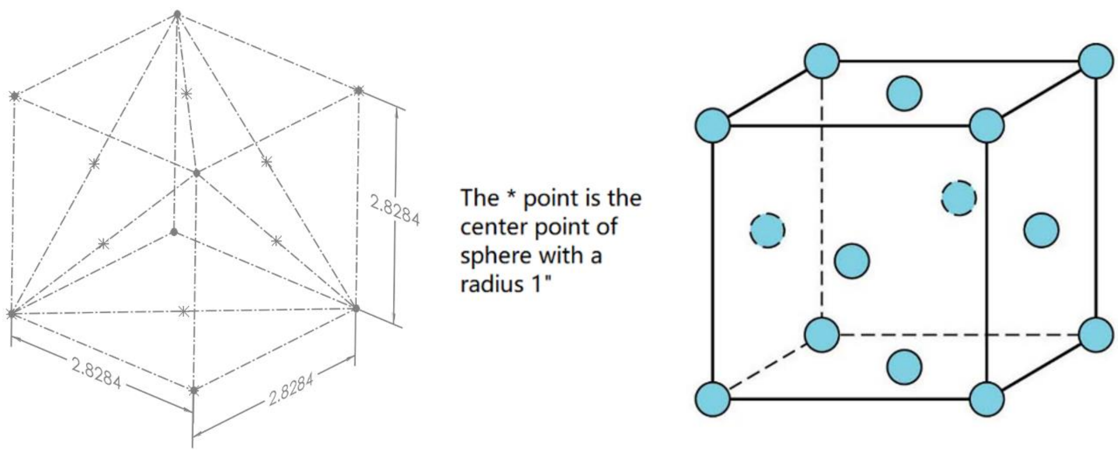


Figure 3 The center points of spheres of the FCC structure

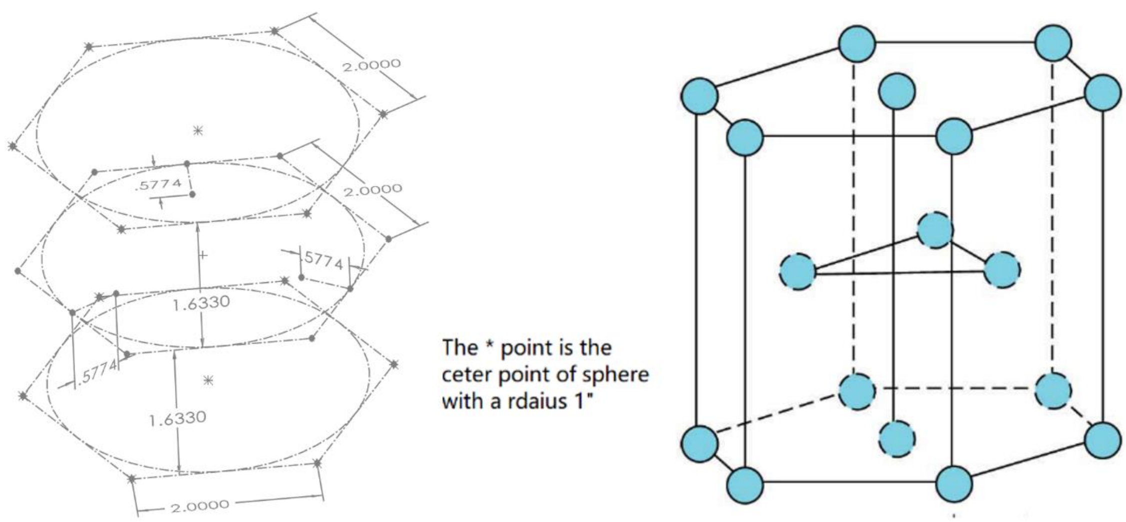


Figure 4 The center points of spheres of the HCP structure

3) In SolidWorks assembly mode, insert the SolidWorks part (the 1" radius sphere) at each center point to create typical BCC, FCC, or HCP crystal structures per the BCC, FCC, and HCP lattices and then use the feature tool "cut-extrude" to convert BCC, FCC and HCP structures into corresponding unit cells. The BCC, FCC, and HCP crystal structure and their unit cells are displayed in Figures 5, 6, and 7. In these figures, the right images are crystal structures and the left images are their unit cells. The purpose of different colors in these pictures is just to make a better visual image.

4) Write and submit a lab report.

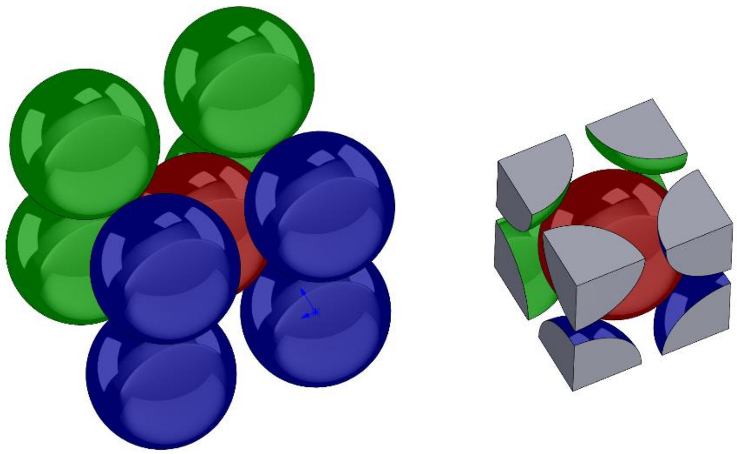


Figure 5 The BCC crystal structure and its unit cell

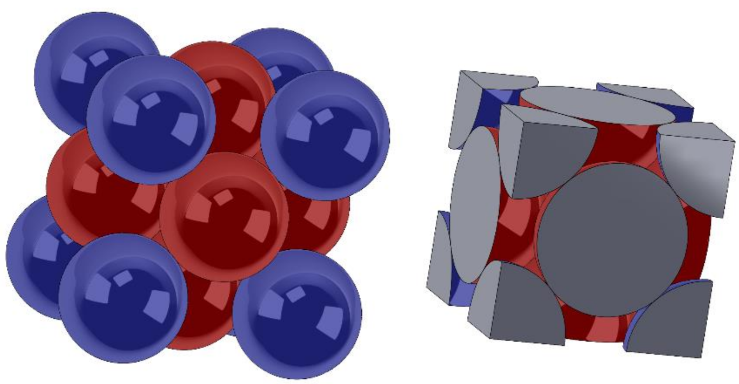


Figure 6 The FCC crystal structure and its unit cell

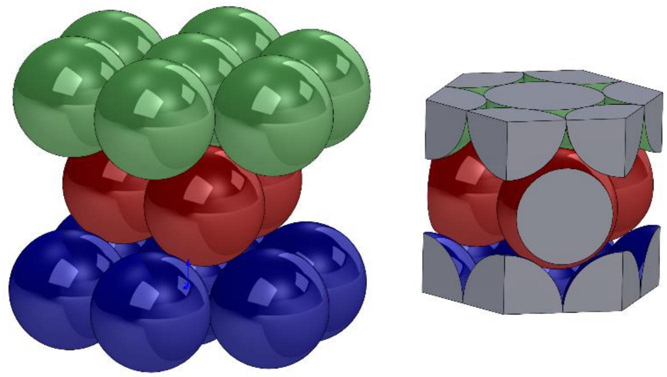


Figure 7 The HCP crystal structure and its unit cell

3.2 PHYSICAL LAB OF TYPICAL CRYSTAL STRUCTURES BY PING-PONG BALLS

The objectives of the physical lab of the typical crystal structure are to study the atomic arrangements of BCC, FCC, and HCP crystal structures with the aid of ping-pong ball representations. Through building the crystal models with ping-pong balls, students will obtain a tangible grasp of the arrangements of atoms in 3D space, and the similarities, and differences among each of the three BCC, FCC, and HCP crystal structures.

Activities of the physical lab of typical crystal structures include the following items.

1) Study and understand the definitions of BCC, FCC, and HCP crystal structures and determine how to use the provided fixtures to build BCC, FCC, and HCP crystal structures. The images of three fixtures are displayed in Figure 8. The "+ sign" fixture is used to help for building the FCC crystal structure. The "X sign fixture is used to help for building BCC crystal structures. The " ✻ sign" fixture is used to help for building the HCP crystal structure.

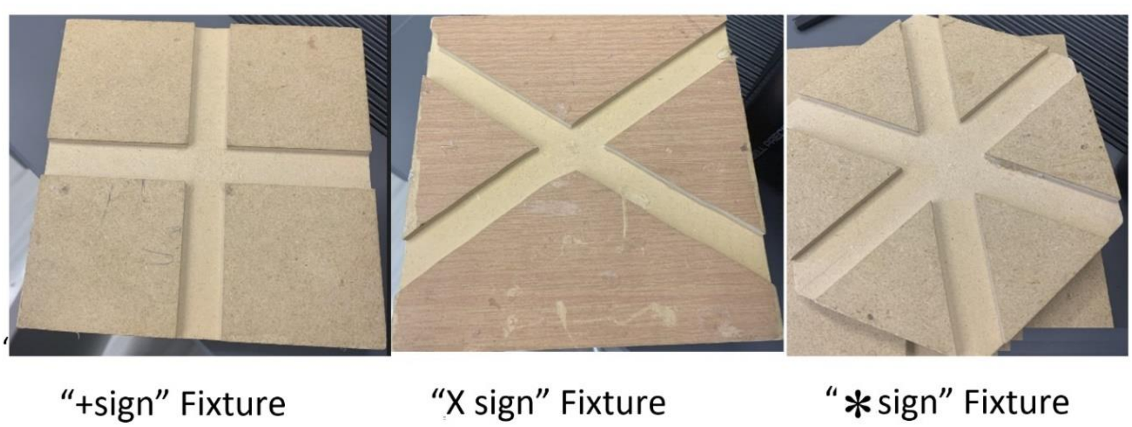


Figure 8 The three fixtures for BCC, FCC, and HCP crystal structures

2) Use the 14 ping-pong balls, plastic glue, and the "+ sign" fixture to build a physical representation of the FCC crystal structure, which is the first image in Figure 9.

3) Use the 9 ping-pong balls, plastic glue, and the "X sign" fixture to build a physical representation of the BCC crystal structure, which is the second image in Figure 9.

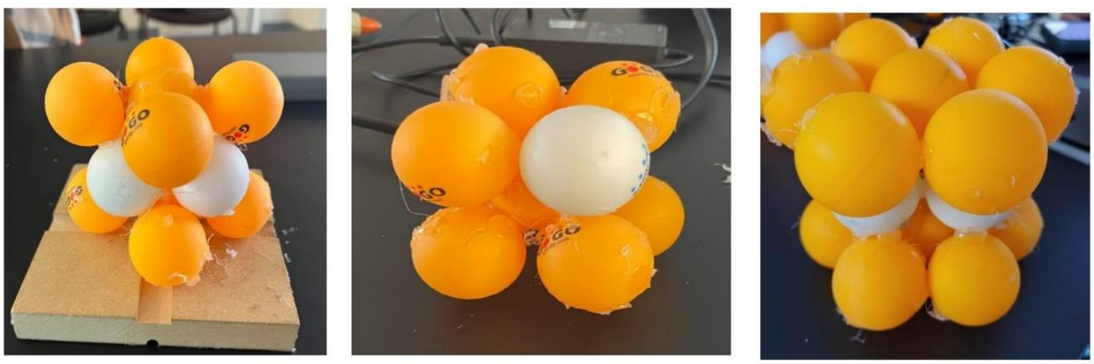
4) Use the 17 ping-pong balls, plastic glue, and the " * sign" to build a physical representation of the HCP crystal structure, which is the third image in Figure 9.

5) Measure the unit cell lattice constants, that is, the side length on the physical models and virtual SolidWorks models and then compare them with theoretical values.

6) Use the measured lattice constants on the physical models and virtual SolidWorks models to calculate the atomic packing factors of each crystal structure and then compare them with theoretical values

7) Study and understand the definition of an octahedral site and then identify & measure the size of the octahedral site on the physical models and virtual models of FCC and BCC crystal structures.

8) Write and submit the lab report



The FCC crystal structure The BCC crystal structure The HCP crystal structure

Figure 9 The physical models of representation of FCC, BCC, and HCP crystal structures

3.3 OBSERVATIONS AND DISCUSSIONS ON THESE TWO LABS

Students worked in a team of four team members. They were asked to study the lab manuals and were encouraged to figure it out first and then to ask for help from the instructors when they had some questions. The followings are some observations and discussions during the labs.

- To make the virtual SolidWorks models for the representation of typical crystal structures, students needed to study and understand the definitions of FCC, BCC, and HCP crystal structures and then build the lattices of these typical crystal structures. Creation and understanding of the lattices of the unit cells in Solidworks helped them to have a better understanding of the arrangements of atoms in typical FCC, BCC, and HCP crystal structures.

- Students were very pleased that they were able to use their SolidWorks skills to create virtual 3D models of representations of FCC, BCC, and HCP crystal structures and used these virtual models to facilitate their understanding of typical crystal structures. The virtual model could be stored on a computer. Students could color the spheres and view the structures at any orientation to get good visual pictures. They could access these virtual models at any time.
- Through the virtual SolidWorks 3D model, students could cut them to get the unit cells and could conduct the accurate measurement of the lattice constant and the size of the octahedral site.
- Even though the physical glued-ping-pong ball representation of typical crystal structures could not present unit cells and could not get accurate measurements, students were still very excited to use the ping-pong balls to build the representation of typical crystal structures. They said that understanding how to use the three fixtures to build a typical crystal structure helped them to have a better understanding of typical crystal structures. They said that the tangible models facilitated their understanding of typical crystal structures.

4. CLASS SURVEY DATA ANALYSIS

To evaluate the effectiveness of the new virtual SolidWorks lab of typical crystal structures, a class survey was conducted. 18 responses out of a total of 20 possible responses were received. The class survey contained four questions and an open comment section.

The survey questions and data results are displayed in Table 1.

Table1 The survey questions and data results

1. The virtual atomic structures experiment using SolidWorks simulation helped me to have a better understanding of the BCC, FCC, and HCP atomic crystal structures.				
strongly agree	agree	no opinion	disagree	strongly disagree
55.56%	27.78%	16.67%	0.00%	0.00%
2. The virtual atomic structures experiment using SolidWorks simulation helped me to have a better understanding of the unit cell and the unit cell parameters of FCC, BCC, and HCP atomic structures.				
strongly agree	agree	no opinion	disagree	strongly disagree
44.44%	44.44%	5.56%	5.56%	0.00%
3. The physical /simulation labs have helped me to better understand the concept of Atomic packing Factor (APF).				
strongly agree	agree	no opinion	disagree	strongly disagree

33.33%	44.44%	22.22%	0.00%	0.00%
4. The virtual atomic structures by simulation were a good addition/compliment to the physical lab.				
strongly agree	agree	no opinion	disagree	strongly disagree
61.11%	33.33%	5.56%	0.00%	0.00%

The followings are the survey results.

- Per the survey results, 83.33% (15 out of 18) students agree and strongly agree that “The virtual atomic structures experiment using SolidWorks simulation helped me to have a better understanding of the BCC, FCC, and HCP atomic crystal structures”. 16.67 % (3 out of 18) showed “no opinion” about survey statement one. No students disagree or strongly disagree with the survey statement one.

- Per the survey results, 88.89% (16 out of 18) students agreed and strongly agreed that “The virtual atomic structures experiment using SolidWorks simulation helped me to have a better understanding of the unit cell and the unit cell parameters of FCC, BCC, and HCP atomic structures”. 5.56 % (1 out of 18) showed “no opinion” about survey statement two. 5.56 % (1 out of 18) of students disagreed with survey statement two.

- Per the survey results, 77.78% (14 out of 18) students agreed and strongly agreed that “The physical /simulation labs have helped me to better understand the concept of Atomic packing Factor (APF).”. 22.22 % (4 out of 18) showed “no opinion” about the survey statement three. No students disagreed or strongly disagreed with survey statement three.

- Per the survey results, 94.44% (17 out of 18) students agreed and strongly agreed that “The virtual atomic structures by simulation was a good addition/compliment to the physical lab”. 5.56 % (1 out of 18) showed “no opinion” about survey statement four. No students disagreed or strongly disagreed with survey statement three.

In a summary, the majority of students agreed that the newly added virtual SolidWorks lab facilitated and helped them to have a better understanding of typical crystal structures and would like to keep it as a good addition/compliment to the physical lab.

The open comment question in the class survey was “ Please provide any additional related comments. Some of the comments are listed below.

- “Overall, I found the labs very insightful as they provided a physical and visual way to interpret the concepts we were learning.”
- “I really liked the Solidworks part of the lab and helped me to better see what the unit cell looks like.”
- “The physical part of the lab helped me learn about the different atomic structures, but the virtual segment felt more accurate and precise.”

- “I feel like the experiment was a good way to learn the subject by physically and virtually creating a model of the unit cells. Two different ways to learn the same topic was good.”
- “I believe the combination of creating the unit cell in Solidworks and building it in class provided a more in-depth understanding than I had gained originally from chemistry class.”
- “Both labs were great in showing each atomic structure. I believe they should be combined as both models were equally effective in teaching the same material.”
- “The physical part of the lab could be improved so that we can get more accurate measurement results which would line up more with the Solidworks models.”
- “These two labs helped me to visualize the different unit cells and the combination of the virtual and physical lab worked very well together.”

5. DISCUSSIONS AND CONCLUSIONS

Typical atomic crystal structures of crystalline solids are important concepts for materials science. Without a good understanding of these typical crystal structures, students will have difficulty grasping the concept of unit cell parameters, atomic packing factor, crystallographic direction, crystallographic plane, tetrahedral site, and octahedral site. It was found that some students still had a hard time developing the spatial thinking skills required to understand typical crystal structures even after they had a physical lab of representation of typical crystal structures and three issues mentioned in the introduction. Since multiple-exposure to the same topics will significantly improve students’ understanding of the topics, we proposed to add a new virtual SolidWorks model for the representation of typical crystal structures to help students to have a better understanding of the typical crystal structures and implemented this new approach last year.

There were two features in this newly added virtual SolidWorks model. The first feature was that to create the virtual models, students must create and understand the unit lattice first by using a 3D sketch in SolidWorks. The second feature was that the virtual models are a 3D representation of the crystal structures. The model can be saved and, viewed in any orientation, and accessed at any time. Upon observations, these two features significantly helped students to have a better understanding of typical crystal structures.

Feedback from students showed that the majority of students agreed that the newly added virtual SolidWorks lab helped them to have a better understanding of typical crystal structures and would like to keep it as a good addition/compliment to the physical lab.

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