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Measuring Student Learning of Crystal Structures Using Computer-based Visualizations

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Abstract

Crystal structures are foundational to many aspects of materials science, yet students often have difficulty visualizing geometric relationships in even the simplest structures. For example, many students make errors when drawing the atomic arrangements on the (110) and (111) planes in the face-centered cubic (FCC) crystal structure. We previously designed an active-learning lesson that allows students to investigate crystal structures and atomic arrangements using a computer program, OVITO. The lesson is designed for a 50-minute introductory materials science course and consists of both individual and group activities. The first part is completed individually and requires students to identify planes and basic crystal structures and then draw and rank the atomic densities of a given set of planes. The second part has students work together in small groups to visualize crystal structures using OVITO, repeating some questions from the first part. Results of the pilot study indicated that the lesson allowed many students to identify and correct mistakes in their initial drawings.

In this work, we categorize and quantify the most common mistakes that students make and investigate errors that seem harder for students to identify and correct. For example, missing atoms are commonly corrected by students, while there are persistent errors in sketching which atoms are (or are not) contiguous. Based on student responses in Fall 2016, we have revised the activity to more clearly emphasize the characteristics of a correct response, and have increased the scaffolding to guide students. Additionally, the revised activity is more focused than the original, allowing students to spend more time on the reflection portion of the activity. Student performance is measured and compared in two courses at different institutions. Student responses on a concept inventory at the beginning and end of the term are also compared to investigate the development and persistence of their learning gains.

1. Introduction

Understanding the three-dimensional relationships in crystal structures is an important skill for materials science and engineering students. However, students struggle to visualize many of the atomic relationships in these three-dimensional structures. For instance, a student may be able to pinpoint the locations of atoms in a unit cell, yet cannot identify which atoms are located on a given plane. A number of interventions have been developed to help students visualize crystal structures, such as using styrofoam spheres or completing computer activities [1]-[4]. One such activity [5] utilizes OVITO [6], an open-access visualization tool used by materials researchers that enables students to visualize crystal structures on their personal computers. The activity is designed to help students learn crystal structures while also improving their computational literacy as they are guided in using OVITO. This learning activity, along with a discussion of its pilot study, was previously reported [5]. A revised version is presented here along with an analysis of student learning.

Overview of Revised Activity

An active-learning module was previously developed to support learning of crystal structures [5],[7]. This two-part activity was based on the ICAP model of learning, which states that learning is enhanced for *interactive* and *constructive* learning experiences [8]. The first part of the activity consists of an individual worksheet that students complete without referencing notes. Students identify Miller indices of planes, sketch planar projections of crystal structures, and rank the planar densities. The second part is a computer-based activity that students complete in small groups. They use provided structure files to visualize crystal structures on their laptops in order to complete a worksheet. Students repeat the sketching exercises, then reflect on their work and note any errors they made in part 1. The activity from Ref. [5] was revised in response to several issues in student responses that were noted in the pilot test. These revisions are summarized in Tables 1 and 2 and discussed in the following sections. Both the first and second versions can be found at Ref. [7].

This activity has been used at several universities in both lower- and upper-division courses. In this paper, we report the results of two studies at different universities. In Study 1, the activity was used in an introductory materials science course, while Study 2 used the activity in a graduate-level computational materials course. The following sections describe the two studies, including the courses, student populations, implementation of the activity, results, and discussion.

Table 1. Summary of the first and second versions of the activity. Italics indicate differences between the versions.

Activity Version 1	**Activity Version 2**

<u>Part 1: Individual</u>
● Identify Miller indices
● Name crystal structures
● For (100) plane:
  ○ Sketch space-filling atoms on plane
  ○ Rank planar density
● For FCC structure:
  ○ Identify Miller indices
  ○ Sketch space-filling atoms on plane
  ○ Rank planar density
● Identify largest planar density for FCC and (100) planes together
	<u>Part 1: Individual</u>
	● Identify Miller indices
	● Name crystal structures
	● For (100) plane:
	  ○ *Sketch (100) plane on provided crystal structure*
	  ○ Sketch space-filling atoms on plane
	  ○ Rank planar density
	● For FCC structure:
	  ○ Identify Miller indices
	  ○ Sketch space-filling atoms on plane
	  ○ Rank planar density
	● *Describe method of ranking planar densities*
	● Identify largest planar density for FCC and (100) planes together

<u>Part 2: Group Work Using OVITO</u>
● Walkthrough using OVITO to slice FCC (110) plane
● For FCC structure:
  ○ Identify Miller indices
  ○ Sketch space-filling atoms on plane
  ○ Rank planar density
● Identify errors in Part 1:
  ○ Correct atoms on planes?
  ○ Correct atoms touch?
● *NaCl structure*
  ○ *NaCl walkthrough*
  ○ *Sketch unit cells*
  ○ *Sketch plane projections*
  ○ *Rank planar density*
  ○ *Compare planar density to FCC*
	<u>Part 2: Group Work Using OVITO</u>
	● Walkthrough using OVITO to slice FCC (110) plane
	● For FCC structure:
	  ○ Identify Miller indices
	  ○ Sketch space-filling atoms on plane
	  ○ Rank planar density
	● Identify errors in Part 1:
	  ○ Correct atoms on planes?
	  ○ Correct atoms touch?
	● *Reflection:*
	  ○ *Describe errors*
	  ○ *What was interesting?*
	  ○ Generate two questions

Table 2. Summary of supplemental materials in versions 1 and 2. Italics indicate differences between the versions.

Version 1	**Version 2**
Survey ● Time to complete activity ● Opinions of activity ● *Reflection:* ○ *What was interesting?* ○ *Generate two questions*	Survey ● Time to complete activity ● Opinions of activity
	Part 3: NaCl Homework (optional) ● *NaCl structure* ○ *NaCl walkthrough* ○ *Sketch unit cells* ○ *Sketch plane projections* ○ *Rank planar density* ○ *Compare planar density to FCC*

Revision: Addressing Incomplete Work

The largest change was shortening the activity since most students were not able to complete both parts of the original lesson within a 50-minute class period. Parts 1 and 2 now contain only metal crystal structures, and the ionic NaCl structure is provided as an optional homework assignment. Reducing the work in part 2 allowed for the reflection questions from the post-activity survey to be included as a part of the activity along with two additional questions. One asks students to describe any errors that OVITO allowed them to catch. This question should enhance metacognition during the activity and prompt students to note their misconceptions. The other question asks students what they found most interesting or eye-opening about the activity, so that they instructor can discover what made the biggest impression on them.

Revision: Targeting Planar Projection Errors

On the first version of the activity, significant errors were noted on the sketches of planar projections on both parts 1 and 2 [5]. However, it was not clear whether students did not read the instructions closely, had poor sketching abilities, or had factual misconceptions. To address this, the instructions to several questions were updated (see Figures 1 and 2). The written instructions now emphasize that students should use space-filling atoms for which nearest neighbors touch. To aid understanding of atomic arrangements on planes, students are first instructed to shade the planes on the 3D images and then identify which atoms lie on the plane (Figure 2).

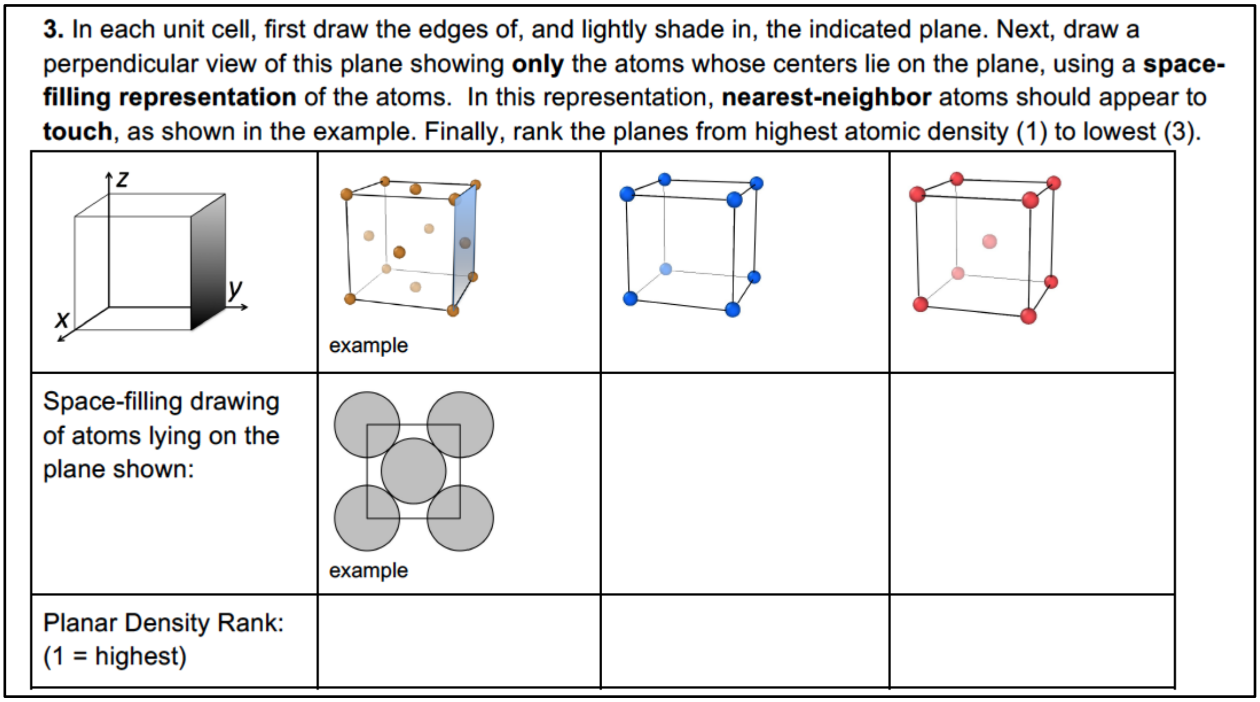


Figure 1. Revised instructions for the (010) planes.

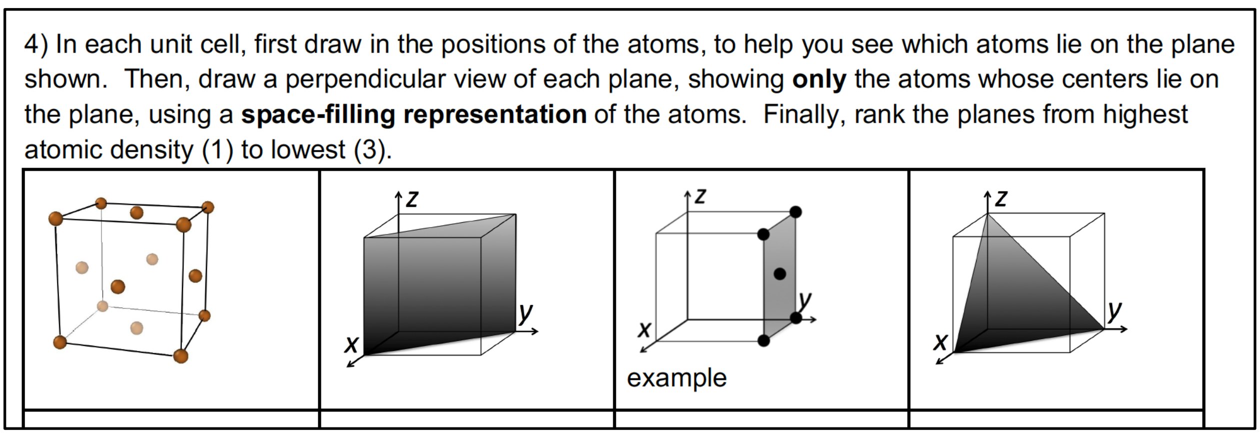


Figure 2. Revised instructions for the FCC planes.

Revision: Articulating Reasoning for Planar Density Ranking

In their individual work, most students in the pilot test were not able to rank the planar densities correctly (<2% in question 3 and 35% in question 4), but few showed any work or provided an indication of the method they used. The new version prompts students: "Describe your method and reasoning for determining the relative atomic planar densities". This requires them to articulate their reasoning and also allows the instructor to see errors in their thinking.

Analysis Guidance

The errors in planar projections were coded for quantitative analysis. We focused on the five types of common misconceptions identified by Krause and Waters: missing atoms, extra atoms, displaced atoms, atoms not touching where they should ("should touch"), and atoms touching where they should not ("should not touch") [9]. An analysis instruction sheet was created to consistently categorize student work among researchers and institutions. The instructions contain examples of correct answers, examples of the misconceptions, and guidelines for consistently coding borderline or ambiguous cases. For example, the 9 locations where atoms should touch on the FCC (111) plane can be divided into 6 "external adjacencies" and 3 "internal adjacencies", as shown in Figure 3. Students may show atoms touching for some but not all of these positions. The guidelines stipulate that a correct answer should have atoms touching for at least 5 external adjacencies and 1 internal adjacency.

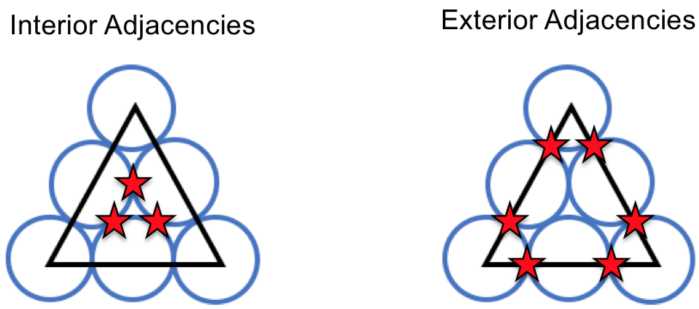


Figure 3. Illustration of the internal and external adjacencies on the FCC (111) plane.

2. Study 1: Introductory Materials Science Course

a. Description of Implementation

Course Description:

Study 1 investigated student learning throughout an introductory materials science and engineering course at a large research institution. This course is primarily taken by sophomore and junior students across the engineering school, and covers common introductory topics such as crystal structures, mechanical properties, and phase diagrams. The course had three fifty-minute lectures each week, as well as a lab component. The course enrollment was 124 students, of whom 68 voluntarily participated in the study.

The instruction of crystal structures was primarily five lectures with occasional active learning. When discussing unit cells, students were presented with images of the simple cubic, FCC, body-centered cubic (BCC), and hexagonal close-packed (HCP) crystal structures, using both the reduced sphere and space-filling representations. A significant amount of instructional time was spent on crystallography and determining Miller indices. The OVITO activity was then completed during one of the 50-minute lecture sessions. Students were not formally instructed about planar density prior to completing the activity. After the module, students were provided with OVITO files for several additional crystal structures (CsCl, NaCl, BCC, and simple cubic) for optional visualization outside of class.

Study Implementation

Student learning and retention was evaluated throughout the course utilizing several different assignments. The study consisted of five parts, which are shown on the timeline of the 30-lecture course (Figure 4). The components of Study 1 are:

- *Concept inventory (initial)*: This assessment included six multiple choice questions on crystal structure visualization.
- *Crystal structure instruction*: As described in the course description (above), students learned about crystal structures in lecture with occasional active-learning activities.
- *OVITO activity (parts 1 and 2)*: The revised activity was implemented in lecture nine. This mirrors the implementation described in our previous work [5].
- *Midterm exam*: One question on the midterm exam asked students to sketch planar projections that they previously sketched in the OVITO activity.
- *Concept inventory (final)*: The concept inventory was repeated at the end of the term.

Throughout these activities, students were repeatedly asked to draw or identify combinations of the FCC and BCC {100}, {110}, and {111} planes. The concept inventory and midterm exam are summarized in the following paragraphs.

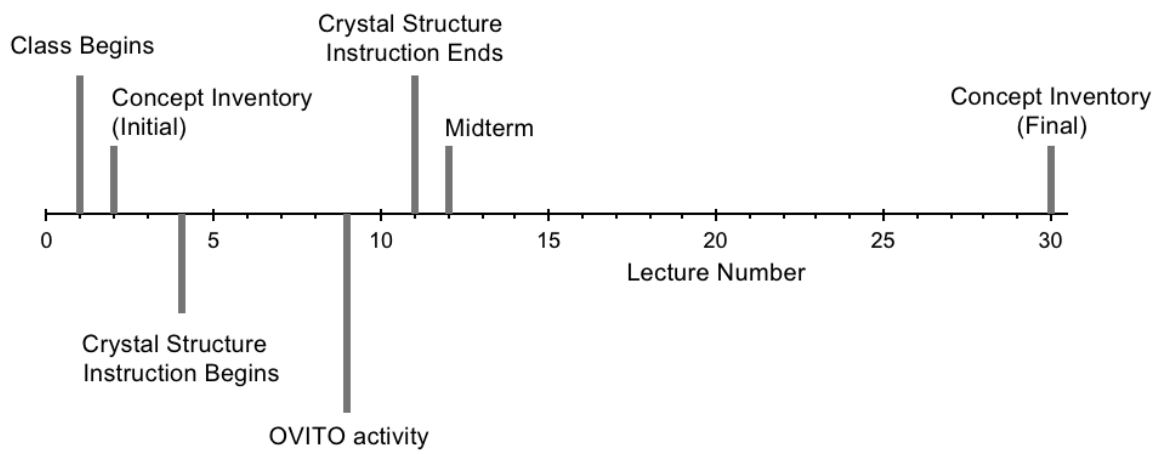


Figure 4. Timeline of Study 1 showing corresponding lecture numbers.

Concept Inventory

A materials science concept inventory was used to assess student learning at the beginning and end of the term. The questions were identical for both concept inventories, but students were not given solutions until after completing the final one. The concept inventories contained 15 multiple-choice questions, six of which were the Crystal Structure Visualization Survey (CSVS) from Krause and Waters [9]. These six questions provided students with images of the BCC and FCC crystal structures and asked students to select the correct planar projection for atoms on the (100), (110), and (111) planes in the BCC and FCC crystal structures. The problem statement for the BCC structure is given in Figure 5, with the multiple choice selections shown in Tables 7 and 8 of the results section.

9-11. For the body-centered cubic crystal structure shown below, choose the correct illustration that shows the atomic arrangement for the specified plane (A, B, C, D, or E). This assumes that the atoms are hard spheres.

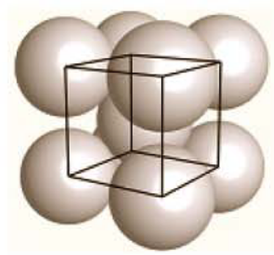


Figure 5. Question prompt for BCC planes on the concept inventory, based on the CSVS.

Midterm Exam

The first midterm exam required students to sketch space-filling representations of atoms on the FCC (110) and (111) planes, which were included in the OVITO activity. As shown in Figure 6, students were required to correctly sketch the shape of the plane, locate the atoms on the plane, and have them touch in the correct locations. Students either had to recall their solution from the OVITO activity or infer the atomic arrangements. Student performance on the exam has not been analyzed to see if there is a testing effect on learning.

c. (6 POINTS) For one unit cell of the FCC crystal structure, sketch the arrangement of atoms on the following planes, using a view perpendicular to the plane and a space-filling representation of the atoms.

(110) (111)

Figure 6. Midterm question on planar projections.

b. Study 1 Results

Sketches of Planar Projections

Student sketches of planar projections were analyzed from parts 1 and 2 of the OVITO activity. On the first part of the activity, which was performed individually without notes, fewer than half of students correctly drew the FCC (110), FCC (111), and BCC (100) planes (Table 3). This indicates that students struggled to visualize structures that were taught in class and that had been included on homework. The specific misconceptions for each plane were tabulated and their frequencies are also included in Table 3, using the five misconceptions identified by Krause and Waters [9].

Table 3. Summary of results in parts 1 and 2 of the OVITO handout in Study 1. The number of students is given on the top line and the fraction of students is listed on the bottom. Fractions can sum larger than 1.00 since some students exhibited multiple errors.
*FCC (100) was included as an example on part 1.

		Correct	**Missing Atoms**	**Extra Atoms**	**Misplaced Atoms**	**Should Touch**	**Should Not Touch**
FCC (100)	**Part 1***	--	--	--	--	--	--
	Part 2 N=56	44 0.79	4 0.07	0 0.00	0 0.00	3 0.05	8 0.14
FCC (110)	**Part 1** N=55	22 0.40	7 0.13	6 0.11	0 0.00	14 0.25	16 0.29
	Part 2 N=58	46 0.78	1 0.02	1 0.02	3 0.05	6 0.10	5 0.08
FCC (111)	**Part 1** N=56	10 0.18	13 0.23	5 0.09	2 0.04	38 0.68	0 0.00
	Part 2 N=55	26 0.47	2 0.04	0 0.00	3 0.05	24 0.44	0 0.00
BCC (100)	**Part 1** N=55	23 0.42	0 0.00	17 0.31	0 0.00	0 0.00	19 0.35
	Part 2	--	--	--	--	--	--

The most common errors are recognizing atoms that should or should not touch. A significant fraction of students also included or excluded atoms, with error frequency dependent on structure. For example, 31% of students included *extra atoms* in the BCC (100) plane and 23% of students were *missing atoms* in the FCC (111) plane on part 1.

In part 2, student performance improved compared to part 1 (Table 3). The gains for the FCC (110) structure were significant. 78% of students correctly drew this plane in part 2, up from 40% in part 1. Students were able to identify *missing* and *extra atoms* when using OVITO, but still had difficulty with *touching* errors. Students made more modest gains with the FCC (111) plane, increasing from 18 to 47% correct. Even after visualizing the atoms on this plane, 44% of students still made significant errors identifying *all* of the atoms that touch. Frequently, students would correctly sketched the exterior adjacencies, but miss the interior adjacencies described in Figure 3.

Ranking of Planar Densities

Two questions in part 1 of the activity asked students to rank planar densities. Almost all students (98%) made errors when asked to individually rank the planar densities of the (100) planes in the FCC, simple cubic, and BCC structures. Most students (93%) were able to rank the FCC (100) higher than the BCC (100) plane, but students frequently ranked the simple cubic (100) plane as having a lower atomic density than the FCC (100) plane, a mistake made by 79% of the students. The only student who completed the question correctly showed mathematical calculations of planar density for each plane. Students performed better on the second set of planar density rankings in part 1, with 33% of students correctly ranking the densities of the (100), (110), and (111) FCC planes.

The revised activity asks students to describe the method they used to rank the planar densities. These methods can be categorized as visual, mathematical, or utilizing prior knowledge, with students using one or more of these components. Some examples of these methods are listed in Table 4.

Table 4. Summary of methods used to determine relative planar densities.

Visual Methods ● "Eyeball" density ● "Eyeball" areas of the planes ● Compare shapes of the planes - square vs. rectangle vs. triangle ● Compare how close the atoms are together/ how packed (in their drawings)
Mathematical Methods ● Count the number of atoms in the plane ● Calculate the area occupied by atoms ● Compute the area of the plane ● Derive the ratio of area occupied by atoms to area of the plane ● Calculate the number of atoms per area of the plane
Utilizing Prior Knowledge ● FCC is "close-packed" ● FCC has highest atomic packing factor

The methods students reported for determining the planar density rankings, coupled with their sketches, provide insight into the sources of error. One common mistake was to incorrectly count the number of atoms on a plane. Fractional atoms at vertices posed the largest problem, particularly for the triangular (111) plane. Another error made by some students was to use volumetric, rather than planar, fractions of atoms. Students also commonly ignored the area of the plane, assuming that all planes had the same area.

The planar sketches greatly impacted the plane rankings, with any errors in the sketches propagating through to the planar density assessments. Some types of errors had a larger effect on the rankings than others. The rankings were particularly impacted by sketches with missing atoms or extra atoms, since the number of atoms on the plane was incorrect. Errors of atoms touching or not touching, on the other hand, affected the area of the plane and seemed to have a smaller impact on the plane rankings.

Despite the multiple challenges to determining the correct ranking of planar densities, student performance improved significantly on part 2. Using OVITO while working in small groups enabled 64% of students to rank the planes correctly, a gain of 31% over part 1.

Tracking Errors Across the Activity

The correlation between individual student responses in parts 1 and 2 was analyzed to identify the extent to which students corrected each type of error. This analysis only includes students who sketched a given planar projection on both parts of the activity; responses to only a single part were omitted. Four specific errors were each exhibited by more than 20% of the students in part 1:

- FCC (111) atoms that “should touch” but did not,
- FCC (111) “atoms missing”,
- FCC (110) atoms that “should touch”, and
- FCC (110) atoms that “should not touch”.

Interestingly, error tracking indicates that in the second part of the activity, some students make *new* errors. Tables 5 and 6 each show two contingency tables for a single error and plane (such as missing atoms on the FCC (111) plane). The contingency tables show the frequencies that the error is absent in both parts, is corrected from part 1 to part 2, persists from part 1 to part 2, or arises as a new error in part 2.

The aggregate data in Table 3 shows that the overall percentage of students who sketch the FCC (111) planes with a “should touch” error decreases from 68% in part 1 to 44% in part 2. Table 5(a), the contingency table for this error, shows information on changes in who is making this error. This table shows that 28% of students made this error in part 1 and were able to correct it in part 2. Another 35% of students made this error in part 1 and did not correct it in part 2. 11% of students made a new “should touch” error in part 2 that was not present in their initial response, and 26% of students did not make this error in either part. Together, the aggregate data along with error tracking in the contingency table indicate that the “should touch” error in the FCC (111) plane is difficult for students to correct.

Table 5. Comparison of the number of students (top number) and fraction (bottom number) in Study 1 with errors in parts 1 and 2 of the FCC (111) plane. (a) "Should touch" misconception. (b) "Missing atoms" misconception.

(a) FCC (111) "Should Touch"

N=46		Part 2	
		Error	No Error
Part 1	Error	16 0.35	13 0.28
	No Error	5 0.11	12 0.26

(b) FCC (111) "Atoms Missing"

N=46		Part 2	
		Error	No Error
Part 1	Error	1 0.02	10 0.22
	No Error	1 0.02	34 0.74

In contrast, the three other common misconceptions in part 1 were well-corrected. Table 5(b) shows that "missing atoms" on the FCC (111) plane were corrected by 22% of students, with only one student (2%) not correcting the error, and one student (2%) showing a new error on part 2. Table 6 shows similar improvements for both "should touch" and "should not touch" errors in the FCC (110) planes. 18% of students corrected their "should touch" errors (8% did not) and 28% corrected their "should not touch" errors (2% did not). For these errors of touching or not touching in FCC (110), very few students developed new errors in part 2, only 4% for each.

Table 6. Comparison of the number of students (top number) and fraction (bottom number) in Study 1 with errors in parts 1 and 2 of the FCC (110) plane. (a) "Should touch" misconception. (b) "Should not touch" misconception.

(a) FCC (110) "Should Touch"

N=50		Part 2	
		Error	No Error
Part 1	Error	4 0.08	9 0.18
	No Error	2 0.04	35 0.70

(b) FCC (110) "Should not touch"

N=50		Part 2	
		Error	No Error
Part 1	Error	1 0.02	14 0.28
	No Error	2 0.04	33 0.66

Concept Inventory: Crystal Structure Visualization Survey (CSVS)

The six questions from the CSVS allow for a standardized assessment of student comprehension of atomic arrangements [9]. Students answered these questions as part of a concept inventory at the start and end of the term. Student performance on these questions is given below in Tables 7 and 8.

Table 7. FCC concept inventory results from the beginning (initial) and end of the course (final). The percentage of students who selected each response (A-E) is indicated, and shading indicates the correct answer. Numbers may not add to 100% due to rounding. Images taken with permission from Ref. [9].

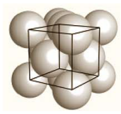
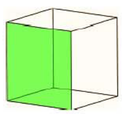
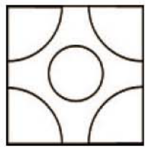
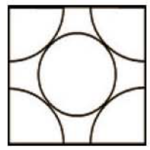
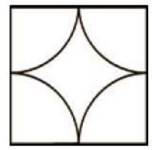
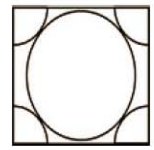
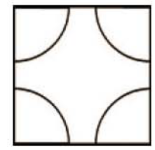
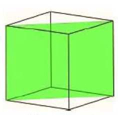
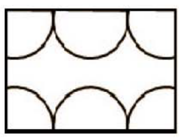
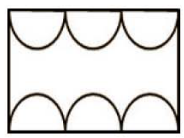
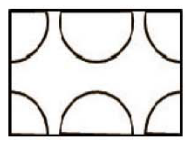
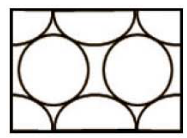
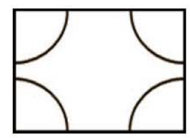
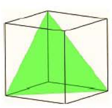
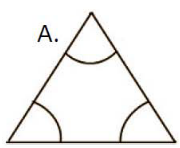
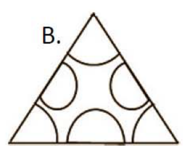
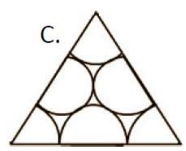
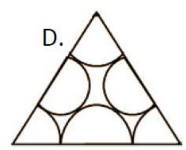
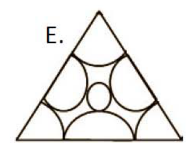
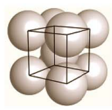
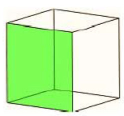
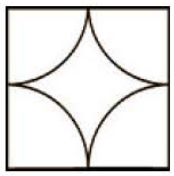
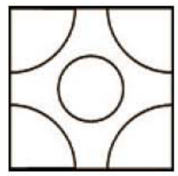
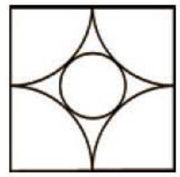
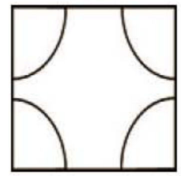
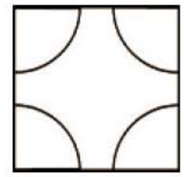
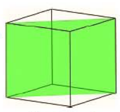
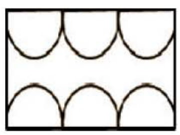
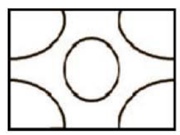
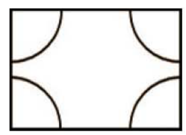
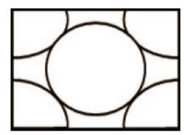
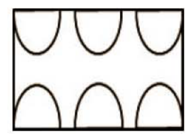
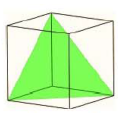
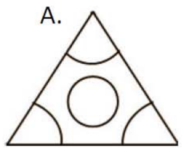
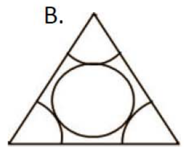
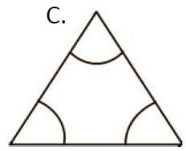
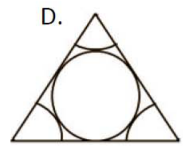
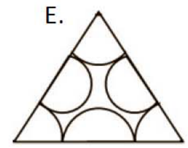
	A	B	C	D	E
 (1 0 0)					
Initial	5%	82%	3%	9%	2%
Final	0%	98%	0%	2%	0%
 (1 1 0)					
Initial	21%	9%	6%	62%	2%
Final	75%	12%	0%	12%	0%
 (1 1 1)					
Initial	3%	9%	49%	29%	9%
Final	2%	2%	66%	30%	0%

Table 8. BCC concept inventory results from the beginning (initial) and end of the course (final). The percentage of students who selected each response (A-E) is indicated, and shading indicates the correct answer. Numbers may not add to 100% due to rounding. Images taken with permission from Ref. [9].

	A	B	C	D	E
 (1 0 0)					
Initial	22%	17%	29%	3%	29%
Final	19%	18%	11%	0%	53%
 (1 1 0)					
Initial	11%	9%	8%	72%	0%
Final	5%	8%	2%	84%	2%
 (1 1 1)	A. 	B. 	C. 	D. 	E. 
Initial	12%	40%	9%	37%	2%
Final	6%	67%	5%	17%	5%

Student learning of the FCC crystal structure was enhanced through the term. The initial and final results in Table 7 indicate that by the end of the course, almost all students correctly placed the FCC (100) atoms. There was an increase of over 50% for students correctly identifying the planar projection of the FCC (110) plane. However, the gain for the correct identification of the FCC (111) plane was more modest, with an increase of only 17% of students over the term.

The concept inventory results from Study 1 and the Krause and Waters study [9] demonstrate that students' planar visualization can significantly improve. Both studies saw the portion of correct responses for the FCC (100) plane increase by similar percentages (16% and 15% for Study 1 and Ref. [9], respectively), although Study 1 had more correct responses on the pretest (70% versus 82%). The results for the FCC (110) plane matched very well between both studies, with 23-25% correct on the pretest and 75% correct on the posttest. However, a notable difference was in the FCC (111) plane. Students from both studies consistently struggled with this plane. Ref. [9] did not see any improvement on this question (47% and 48% on the pretest and posttest, respectively), whereas there was an increase of 17% in Study 1 (from 49 to 66%). However, a large fraction of students were still unable to identify the correct structure at the end of the quarter.

In contrast to the improvement in recognizing FCC planes, Table 8 shows that student performance on the BCC crystal structure improved only slightly over the term. Although the amount of correct responses for the (100) plane increased, at the end of the quarter still only half of students were able to correctly identify this planar arrangement. Student performance for the BCC (111) plane was very poor at the beginning of the term and slightly *decreased* at the end of the term, with many students maintaining the misconception that the body-centered atom (located at a position of ½ ½ ½ in the unit cell) lies on the (111) plane. Student learning of the BCC crystal structures in this study did not improve as much as that for the students in the study of Ref. [9]. In that study, there was a significant improvement on student responses for the BCC (100), (110), and (111) planes, increasing from 40% to 83%, 67% to 95%, and 9% to 35%, respectively.

c. Discussion of Study 1

The learning gains across the term were measured through both the CSVS concept inventory and the OVITO activity. We were particularly interested in whether learning gains would persist over the quarter or if student responses only improved when completing handouts alongside the structure visualizations. As shown in Figure 7, the percentages of correct responses generally increased over the quarter. Instruction on the topics during the time between the initial CSVS and part 1 of the OVITO activity resulted in modest learning gains for the FCC (110) and BCC (100) planes. The percentage of correct responses dropped for the FCC (111) plane, which could be attributed to the difference between answering a multiple choice question and the more open-ended problem of accurately sketching a plane.

Student performance on the FCC (110) structure improved significantly during the OVITO activity, and much of this improvement persisted to the end-of-term CSVS. Student performance on the FCC and BCC (100) planes showed a smaller improvement over the term, which is not surprising, as the OVITO activity did not emphasize these planes. After the initial drop in performance, the fraction of correct student responses for the FCC (111) plane rebounded in the OVITO activity, and improved slightly more at the end-of-term CSVS, ending modestly higher than the initial fraction correct at the beginning of the term. Evaluation of the types of errors indicates that students continually respond with answers in which not all of the FCC atoms in the plane touch where they should.

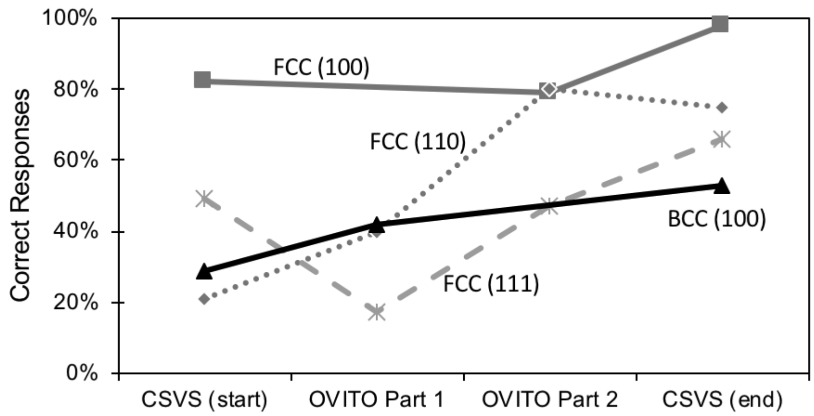


Figure 7. Accuracy of student responses on the four assessments tracked over the term, for all four planes included on the CSVS.

3. Study 2: Graduate-Level Computational Materials Course

a. Description of Implementation

Course Description

Study 2 took place in an early graduate/advanced undergraduate course in physics/materials science and engineering/computational science at different large research institution. This course is primarily taken by senior undergraduate and first-year graduate students. The majority of students are in physics or materials science and engineering, but some come from other departments including bioengineering and computer science. Hence, students' prior experience with materials science and crystal-structure analysis ranges from none to an advanced undergraduate-level of exposure.

The course does not explicitly cover crystal structures. Topics covered in the course include classical techniques for computing thermodynamic properties and behavior on an atomistic length scale, such as Molecular Dynamics and Monte-Carlo simulations. The course had two eighty-minute lectures each week. The course enrollment was 42 students, of whom 38 voluntarily participated in the study. The OVITO activity was completed during one of the 80-minute lecture sessions, in preparation for a team-based simulation project, for which some of the students chose OVITO as a visualization and analysis tool. Students were given approximately 25 minutes for part 1 and 40 minutes for part 2, and appeared to have had enough time to complete the activity.

b. Study 2 Results and Comparison to Study 1

Sketches of Planar Projections

As in Study 1, student sketches of planar projections were analyzed from parts 1 and 2 of the OVITO activity. The results are summarized in Table 9, including frequencies of the five misconceptions.

Table 9. Summary of results in parts 1 and 2 of the OVITO handout in Study 2. The number of students is given as the top number, with the fraction of students given on the bottom. Fractions can sum to more than 1.00 since some students exhibited multiple errors. *FCC (100) was included as an example on part 1.

		Correct	Missing Atoms	Extra Atoms	Misplaced Atoms	Should Touch	Should Not Touch
FCC (100)	**Part 1**	--	--	--	--	--	--
	Part 2 N=38	28 0.74	3 0.08	0 0.00	2 0.05	6 0.16	1 0.03
FCC (110)	**Part 1** N=38	20 0.53	7 0.18	2 0.05	3 0.08	8 0.21	7 0.18
	Part 2 N=37	25 0.68	2 0.05	2 0.05	3 0.08	7 0.19	1 0.03
FCC (111)	**Part 1** N=37	13 0.35	3 0.08	4 0.11	2 0.05	19 0.51	0 0.00
	Part 2 N=38	23 0.61	1 0.03	1 0.03	1 0.03	14 0.37	0 0.00
BCC (100)	**Part 1** N=38	28 0.74	0 0.00	3 0.08	0 0.00	0 0.00	7 0.18
	Part 2	--	--	--	--	--	--

Overall, the advanced students in Study 2 performed comparable to or better than the introductory students in Study 1, except with the FCC (110) plane in Part 2. Student performance improved when completing the OVITO activity for both the FCC (110) and FCC (111) planes. Student misconceptions decreased from parts 1 to 2. On the second part, the frequency of most errors was less than 10% on part 2. A notable exception was the “should touch” error, which was very common across planes and more persistent than other errors. This error was the most common for the FCC (100), which is surprising since students were provided with a correct figure in part 1. Additionally, students were specifically instructed to use a space-filling representation of atoms.

We propose that a new type of error should be included in the analysis: that of using the reduced sphere representation even when instructed to use a space filling representation. This error applies to sketches where atoms are not touching (as expected) but are too far separated. For example, atoms on the BCC (100) plane should not touch, but they should be separated only slightly, enough to accommodate the body-centered atom. Using this new category, the two most common errors for the BCC (100) plane in Study 2 were atoms that "should not touch", and "reduced sphere", each occurring at a rate of 18%. We also see "reduced sphere" errors for the FCC (100) plane despite instructions to use a space-filling representation of atoms, the example provided in part 1, and the visualization in OVITO.

Although the "reduced sphere" misconception was not included in the initial analysis in Study 1, we expect both populations to demonstrate similar misconceptions. Including the "reduced sphere" error for BCC (100) in Study 1 makes this the most common error, made by 33% of the students. Atoms that "should not touch" was the next most common error made by the introductory students in Study 1 for BCC (100). This error implies that students did not take into account the effect of the volume of the body-centered atom on the spacing of the atoms on the BCC(100) plane.

Ranking of Planar Densities

In Study 2, 16% of the students were able to correctly rank the planar densities of the (100) planes in the FCC, SC and BCC structures in part 1. This is a very low rate, but higher than the introductory students (2% correct in Study 1). All but one of the students with a correct planar ranking showed detailed mathematical calculations of planar density or area ratio of atoms for each of the three planes. Compared to the novice students in Study 1, a greater percentage of the advanced students in Study 2 carried out mathematical calculations in their approach to this problem.

In both studies, correct rankings on part 1 were supported by mathematical calculations, with only a single exception. If the geometric calculations are not performed, students will likely rank these planes incorrectly. The FCC (100) and BCC (100) planes are easier to deduce, with 93% and 95% correct responses in Study 1 and Study 2, respectively. However, the FCC (100) and simple cubic (100) planes must be calculated.

The second planar density ranking was for the FCC (100), (110) and (111) planes in question 4. In part 1, 68% of the students in Study 2 answered this question correctly. Few students (8 /38) showed complete geometric calculations, but this fraction is still higher than in Study 1. Many students combined visual methods with calculations, such as writing the equation for planar density and counting atoms, but not performing the calculation. One student expressed this method well, "Projection on the plane shows 2 atoms per plane on *all of them*. But the (110) plane seems to be the biggest area, so the least density. The FCC plane (111) seems to be the least area [*sic*] than the (010) plane so the (111) plane should be the most dense." Interestingly, group work using OVITO did not aid students, as only 69% correctly answered this on part 2. The novice and advanced students in the two studies completed the second part with similar accuracy. It is unclear why the advanced students did not improve on this activity, but it is hypothesized that the rankings are hindered by persisting errors in drawing the planes.

Tracking Errors Across the Activity

Students in Study 2 persistently had difficulties sketching the FCC (111) plane. The primary misconception was that sketched atoms “should touch” but do not. Only 49% of students did not have this error on the FCC (111) plane in part 1, with Table 10(a) showing how the errors are correlated between parts 1 and 2. While 27% of the students made this error in part 1 and were able to remedy the error in part 2, 24% of students had a persistent error. 14% of responses had new errors that were not present in part 1. Comparison with Table 5(a) shows that the students in Study 2 had behavior more or less comparable to those in Study 1 for the fractions of students who are able to identify errors or create new errors. However, comparison of Tables 5(b) and 10(b) indicates fewer students in Study 2 had the “missing atom” error on the FCC (111) plane, as compared to Study 1. The “missing atom” errors in Study 2 are all new errors, but this could be insignificant due to the small sample size. The reduced error prevalence in Study 2 is likely because advanced students have had more experience with crystal structures.

Table 10. Comparison of the numbers of students (top number) and fractions (bottom number) in Study 2 with errors in parts 1 and 2 of the FCC (111) plane. (a) “Should touch” misconception. (b) “Missing atoms” misconception.

(a) FCC (111) “Should Touch”

N=37		Part 2	
		Error	No Error
Part 1	Error	9 0.24	10 0.27
	No Error	5 0.14	13 0.35

(b) FCC (111) “Atoms Missing”

N=37		Part 2	
		Error	No Error
Part 1	Error	0 0.00	3 0.08
	No Error	1 0.03	33 0.89

A substantial fraction of advanced students had “should touch” errors with a low rate of remediation for the FCC (111) plane. We hypothesize that this is because the reduced-sphere representation is commonly used in literature. Experts understand that certain atoms touch, even when the atoms are not shown as touching in their drawings. Notably, some of the students in Study 2 who showed work for planar density calculations and ranked the FCC (111), (110), and (100) planes correctly, used the reduced sphere representation in some or all of their drawings. Despite using this representation, which results in a “should touch” error, these students have a correct understanding of the geometric relationships in the unit cell. They simply chose not to draw space-filling atoms, despite the instructions for the activity.

For comparison to Study 1, the persistence of “should touch” and “should not touch” misconceptions were evaluated for the FCC (110) plane. Table 11 shows these errors were readily remedied in part 2, consistent with Study 1 results in Table 6. The FCC (110) “should not touch" error was remedied by all students who made the error in part 1, while the "should touch" error persisted for 14% of the students. Again, it is unknown whether some of these students chose to use the reduced-sphere representation.

Table 11. Comparison of the number of students (above) and fraction (below) in Study 2 with errors in parts 1 and 2 of the FCC (110) plane. (a) "Should touch" misconception. (b) "Should not touch" misconception.

(a) FCC (110) "Should Touch"

N=37		Part 2	
		Error	No Error
Part 1	Error	5 0.14	3 0.08
	No Error	2 0.05	27 0.73

(b) FCC (110) "Should not touch"

N=37		Part 2	
		Error	No Error
Part 1	Error	0 0.00	7 0.19
	No Error	1 0.03	29 0.78

4. General Discussion

Fixing Misconceptions

Throughout the studies, certain misconceptions were easier for students to correct than others. The pilot study noted that students struggled to correctly sketch the atoms that touch, particularly with the FCC (111) plane [5]. Our hypothesis was that students' poor sketching abilities was the source of this error. This led us to update the directions to explicitly emphasize the use of space-filling representations so that it is clear where the atoms touch. However, there were still significant errors with the revised activity. For the "should touch" misconception on the FCC (111) plane, some students correct their errors when completing part 2 of the activity, but 11% of novice students had new errors (Table 5(a)). This error persists for a significant fraction of students, as only 47% and 66% of students had correct responses to OVITO part 2 and the final concept inventory, respectively. The poor results on the concept inventory indicate that students continue to have errors identifying atoms that should touch or not touch, even when sketching ability is not a factor.

For the advanced students in Study 2, the source of the "should touch" errors on the FCC (111) plane are not known. For some students, their sketches seem to indicate that they used the reduced-sphere representation, which could be the source of the error. However, this has not been verified. In the future, the CSVS questions could be used to confirm that students understand the geometric relationships while minimizing the importance of reduced-sphere/space-filling representations or sketching ability.

The activity is more successful at helping students identify missing or extra atoms. Students consistently fixed these errors from part 1 to part 2 of the activity. This is supported by results of the concept inventory in Study 1. For example, 62% of these students initially thought that the

FCC (110) plane had atoms in the center, not only around the edges. This "extra atom" misconception dropped significantly by the end of the quarter, as only 12% of the students selected the incorrect answer. Similar success was achieved with these errors for students in Study 2. Notably, this error is not dependent on using the space-filling representation.

Ranking Planar Density

Students' planar density ranking was significantly supported by the new prompt to explain their reasoning. This question alerts students that there should be a method for this task, and requires them to think critically to perform the calculation. Many students showed evidence of counting atoms and fractional atoms, with a few calculating areas of the planes. By contrast, in the pilot study from Ref. [5], very few students had any markings on the page that showed either counting of atoms or any calculations of areas. Those students made errors in the rankings, without any indication about the sources of their misconceptions.

Although students are using more sophisticated thought-processes with the revised instructions, the ranking tasks continue to be challenging. One explanation for the low improvement in correct planar density rankings in Study 1 is that cascading errors, starting with the large number of incorrect drawings in part 1, made it likely for students to propagate errors in their evaluations of planar densities. The students might use the correct method, but their inputs to the calculation (number of atoms, plane dimensions, etc) are incorrect. A significant gain is seen in part 2, where 82% of students in Study 1 ranked all three planes correctly, compared to 64% of students in the pilot. In Study 1, since students first worked individually on ranking planar density, they entered the interactive part of the activity with a specific method to discuss with others in their group.

Reflection: Identify Any Errors?

As a metacognitive task, students were prompted to compare their results from parts 1 and 2 and identify any errors that were corrected. 88% of students in Study 1 noted errors in their sketches from part 1 to part 2. Many of the comments discussed the touching and spacing of the atoms, particularly on the (111) FCC plane. For instance one student wrote "my (111) sketch left empty space in the middle, so my density evaluation was off." The students in Study 1 were self-aware of their novice abilities and were able to identify some of their own misconceptions. In contrast, the students in Study 2 were overconfident about their performance. 61% reported that there were no errors for any of the sketches. However, only 35% correctly sketched the FCC (111) drawing on part 1! Of the students who reported "no errors", they were nearly evenly split between correct and incorrect images. Only 29% of students had correct sketches and reported no error, while 31% responded there was no error despite having one or more incorrect sketches. It is likely that these advanced students were not careful in their sketches or lacked the metacognitive ability to judge the correctness of a response (such as atoms touching in the correct locations with the space-filling representation).

Reflection: What was Interesting?

In addition to analyzing their own errors, students were asked to reflect on the activity and consider what they found "interesting or eye-opening". Responses to this question were positive, with many comments mirroring their course content and their level of experience. The OVITO activity had something interesting to offer to students in both introductory lower-division and graduate-level courses.

In Study 1, students reported many things about the crystal structures that were interesting. Several students were surprised by how closely packed the FCC (111) plane is. The geometry of atom arrangements surprised them in different ways. One student wrote "atoms do touch, after all", while another noted how atoms on some planes do not touch as much as expected. Students liked OVITO's visualization capabilities, specifically the ability to see structures and planes from different perspectives and the potential to visualize more complicated structures.

In Study 2, fewer students commented on features of the specific crystal structures used in the activity, but they were interested in the application of OVITO to structures in general. They liked the quality of the graphics, ease of use and ability to "move around" the structure with a few mentioning the slice function in particular. They noted the ability to visualize complex crystal structures and simulations. A few mentioned that crystallography was new to them, and interesting. Several talked about special features in OVITO, such as labeling atoms according to properties and being able to do things automatically. A couple students said that OVITO would be useful for their research.

Reflection: Generate Questions

The final reflection question asks students to "generate at least 2 questions you have about structures of materials or how we visualize or work with them". Students in both courses asked a wide range of questions, many of which focused on recent course topics. These responses are given in Appendix A, but can be separated into the following categories:

- Procedures related to the activity,
- Crystal structures,
- Structure-property relationships,
- Modeling crystal structures, and
- Using OVITO.

The responses to this question were very indicative of the course content. Novice students in Study 1 asked significantly more questions related to crystal structures, mechanical properties (which are covered in the course) and methods to answer the questions on the worksheet. For example, two questions were "How to check [planar] density easier" and "How would different structures affect strength." In contrast, students in Study 2 asked more questions related to OVITO's functionalities and use with simulations. Students wanted to know "What are real-life applications of OVITO" and whether OVITO can visualize electron density/defects/ dislocations/etc. The student responses provide insight into the directions taken by students' curiosity; several could serve as nice segues to upcoming course topics, such as the questions relating to structure-property relationships for Study 1 or the use of OVITO with simulations for a course project in Study 2.

5. Conclusions and Future Work

An active-learning activity for visualizing crystal structures was studied in two classes at different institutions. Student learning of crystal structures increased for both the introductory course (Study 1) and the advanced course (Study 2) when completing the activity. The learning was most enhanced for the FCC (110) planar projections, as many students corrected misconceptions of atoms which should and should not touch. However, other plane/misconception pairs were much more difficult to correct, such as "should touch" errors on the FCC (111) plane. Finally, we found a new error which arose when completing the activity, indicating that comprehension of planar projections is more complicated than only fixing existing misconceptions.

There is a need to develop targeted activities for persistent errors that are difficult for students to fix. Two particularly troublesome misconceptions are atoms not touching on the FCC (111) plane and extra atoms on the BCC (111) plane. For these planes, we suggest developing questions which emphasize these misconceptions. For instance, the BCC (111) plane can be shown with reduced-sphere atoms, then students can use OVITO to rotate the structure in all directions to see that the body-centered atom lies *above* the (111) plane. For the FCC (111) atoms, students can be prompted to identify all the adjacencies, both on the exterior and interior of the plane. A new, targeted activity would allow students to focus their efforts on the misconceptions that are particularly challenging to overcome.

Finally, the activity can be modified to fit the needs of a specific class, whether it is an introductory or advanced class. This activity was originally designed for an introductory course, which needs additional practice in identifying crystal structures and Miller indices. However, these items can be removed if an instructor would like to emphasize other aspects of crystal structures. Using reflection questions, such as having students generate their own questions, can provide an instructor significant insight into modifying the activity for their own class. For the introductory students, whose questions focused on the basics of atomic structures, future revisions can emphasize atomic packing. In contrast, upper division students can use this activity to explore some of the functionalities of OVITO, such as analyzing other data sets or using additional capabilities of the software. Although this activity has been designed for instructors to use as-is, it also provides significant opportunities for tailoring learning to the needs of the students.

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Appendix A. (a)-(e) Selected student responses to reflection question for Studies 1 and 2.

(a) Calculations and procedures related to the activity handout
Study 1 ● How do you know how to space atoms? ● How can you tell which atoms lie in indicated planes? ● How to check density easier? ● Why did we change the distance?

(b) Crystal Structures
Study 1 ● What significance does the structure [have]? ● [How are bonding and structure related?] ● Why don't atoms touch as much? ● How do ratios of atoms change structure? ● How the CN affects the different structures ● How do we know without simulation which direction is closely packed? ● What other common planes are there? ● What's the most atom we can put in crystal structure? ● Are there structures of materials that have yet to be determined? ● Do polymers also have this cubic structure, even though they are long strands?
Study 2 ● How does interplanar spacing vary as a function of planar density? ● What determines the equilibrium structure of a material?

(c) Structure-Property Relationships
Study 1 ● How bonding types relate to density? ● Are there innate properties dependent on crystal structure, if so, why? ● How would different structures affect strength? ● I would like to compare [bond strength of] the FCC and BCC structures to the simple cubic. ● Does higher planar densities in some directions mean that materials exhibit planes of higher and lower strength?
Study 2 ● Can crystal structures affect magnetic/ optical properties? ● How does crystal structure affect self-assembly of materials?

(d) Modeling Crystal Structures
Study 1 Questions ● Why do we use hard spheres? ● How good of an approximation is the hard sphere model when it comes to actual usage?
Study 2 Questions ● How accurate is a representation that relies on an approximate atomic radius? ● How realistic or useful is it to use visuals where atoms are touching w/ each other.

(e) OVITO Use, Capabilities, Limitations
Study 1 Questions ● How do you make 3D models? ● How to visualize hcp structure? ● Are the structures with their measurements exact or have a certain tolerance? ● The (111) view was weird, how do I make it more clear in OVITO? ● Are the structures with their measurements exact or have a certain tolerance? ● Can we visualize the density?
Study 2 Questions ● How do you generate more complex structures? ● What are real-life applications of OVITO? ● How does OVITO benefit research? ● How can MD results be visualized with OVITO? ● Can OVITO visualize: [electron density, defects, dislocations, interstitial sites]? ● Why OVITO over VMD? ● Have you used the python scripting with OVITO for structure generation?