Paper ID #20127

A Computer-Based Interactive Activity for Visualizing Crystal Structures in Introductory Materials Science Courses

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Abstract

This paper presents and discusses an interactive classroom activity on visualizing the atomic arrangement of common crystal structures and planes. This two-part module is built upon the ICAP framework [1], with students first completing an individual *constructive* activity, where they mentally visualize and manipulate crystal structures. The second part is an *interactive* activity in which students work together to view and manipulate crystal structures using OVITO, an open-source software tool. At the end of the exercise, students evaluate their previous individual work using the solutions from the group. This lesson both challenges students to synthesize information about crystal structures and introduces them to a visualization tool used by researchers. The module was pilot-tested in a fifty-minute lecture of an introductory materials science course at a large research institution. Students downloaded and ran the software on their personal computers, which most students found to be reasonable. Students perceived this activity to be useful and educational, and preliminary results indicate that the activity supported student learning. Samples of student work are included to illustrate misconceptions that were identified and corrected during the activity. All of the resources for this activity are shared publicly to support other faculty in their curricular innovations.

1. Introduction

A cornerstone of materials science and engineering is the composition-structure-processing-properties paradigm that guides the design and analysis of materials. Crystal structures play a critical role in determining the properties of materials and are often introduced early in materials science courses, prefacing the structure-property relationships that are covered subsequently. It is important to understand the geometric relationships of atoms in crystalline structures, such as the coordination number and the atomic arrangement on close-packed planes. However, students often have difficulty visualizing structures [2], which can lead to errors in determining other important geometric features in the crystal.

Student misconceptions of crystal structures were previously investigated by Krause and Waters [2]. They studied students' ability to correctly sketch or identify the atomic arrangement of the (100), (110), and (111) planes in body-centered cubic (BCC) and face-centered cubic (FCC) crystal structures. They identified 5 common types of misconceptions that arose in this activity: 1) Missing atoms, 2) Extra atoms, 3) Misplaced atoms, 4) "Non-touching atoms where they should touch", and 5) "Touching atoms that should not touch". The authors quantified the types of misconceptions for each plane, and found that students' difficulties increased going from the (100) to the (110) to the (111) planes, for both FCC and BCC structures. Krause and Waters' results show that the majority of students are unable to visualize and sketch all of these planes correctly before instruction, with some still experiencing difficulty after instruction. Their work indicates that instruction is capable of ameliorating misconceptions, but that targeted activities would be helpful to improve students' understanding. Furthermore, their work provides an assessment that can be used as a metric for identifying and quantifying student errors and evaluating the success of targeted interventions.

1.1 Teaching Crystal Structures

Crystal structures have been the focus of a variety of educational activities, demonstrations and tools. Several papers have presented activities utilizing physical spheres, such as latex balls [3] or marbles [4], to build crystal structures. These activities aid students' visualization skills, allowing them to physically manipulate atoms rather than relying on spatial reasoning. However, these activities are limited in the types of views and planes that can be visualized, and are also difficult to scale to large-lecture situations. One alternative is to use the plan view, which shows specific slices through a unit cell and provides information about crystal symmetry [5]. This clarifies atomic positions for students, but does not allow students to visualize any plane of their selection.

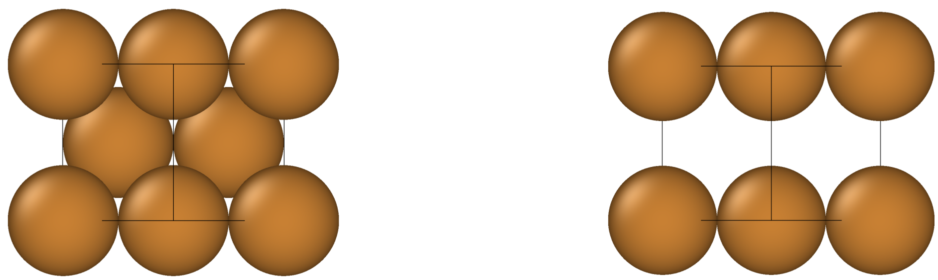
Computer-based activities can provide students with more flexibility in manipulating structures. In 1996, Foley [6] developed a computer program, CrystalVis, to teach students about crystal structures with a focus on crystallographic notation and crystal symmetry. Since then, other software programs have been developed to visualize crystal structures, such as CrystalMaker [7] and Luealamai and Panijpan's computer game on unit cells [8]. However, many of these programs either require a licensing fee or are not research-grade tools. Furthermore, many existing publications on crystal structure activities do not provide a strong pedagogical basis for the activity design nor do they report specific learning gains. Work is needed to develop crystal visualization learning activities that are grounded in educational theory and that utilize widely-used, modern computational tools.

1.2 Teaching Computational Tools

Engineering students should be introduced to computational tools used by the professional materials science community to develop their computational literacy, a skill that is becoming increasingly important for the development of a modern workforce. The 2011 Materials Genome Initiative called on scientists and engineers to revolutionize materials development by integrating experiments, digital data, and computational tools [9]. Furthermore, industry [10], the National Science Foundation [11], and the National Research Council [12] have all identified enhanced instruction of cyberinfrastructure concepts and preparing "technologically agile" [11] students as vital for a modern engineering workforce. Thus, it is important to incorporate computational tools in the materials science curriculum [13], and many universities are adding these tools to existing courses or revising entire course sequences to teach students more computational skills [14-16].

One important computational visualization tool for research and teaching is the Open Visualization Tool, OVITO [17, 18]. This open-source software program visualizes and analyzes 3D materials structures as well as time-dependent output from molecular dynamics (MD) and Monte Carlo (MC) simulations. It is free to use and available on the most common computer platforms. OVITO's analysis tools include analyzing common neighbors, calculating atomic displacements, and classifying dislocations and partial dislocations within a structure. OVITO's research capabilities have been well demonstrated, as the seminal article [18] has been cited over 1000 times [19]. OVITO has also begun to be used as an educational tool. For example, the

University of Illinois at Urbana-Champaign uses OVITO in their computational materials science curriculum [16]. In the activity reported here, OVITO is utilized to help students visualize crystal structures and manipulate unit cells, producing images such as those shown in Figure 1, of the FCC unit cell sliced on the (110) plane.



A **B**

Figure 1. Projection view of the (110) plane in an FCC crystal structure, created and displayed using OVITO. Atoms are scaled to be space-filling, and the unit cell outline can be displayed or hidden. Figure 1A shows a view of the (110) plane, including atoms in the unit cell that lie behind the plane. Figure 1B shows a sliced view of the (110) plane, displaying *only* the atoms whose centers lie on the (110) plane.

The authors designed a classroom activity to enhance the teaching of crystal structures while also increasing students' computational literacy. This introductory-level activity engages students in learning crystal structures and guides them in using the tool OVITO. The activity is informed by educational research on effective classroom activities. Furthermore, the activity is designed to be accessible to other instructors and students, so the following constraints are imposed: the activity should be implementable in a lecture-hall setting, within the traditional lecture time-frame with no need for a studio or lab environment; instructions are sufficient so that the instructor does not need prior experience with OVITO; internet access during the activity is not required; and no special equipment or supplies are needed. The visualization activity is completed in small groups, and since many students own laptop computers, there are sufficient computers utilizing only those that are brought to class.

2. Activity Design

2.1 Theory

Educational research has consistently provided strong evidence that student-centered, active-learning techniques are more effective at promoting deep student learning than traditional lecture-based methods [20]. One such method of structuring student learning is through the ICAP framework [1], which provides a method of relating types of learning activities to their associated learning gains. The ICAP framework categorizes student engagement behavior into four modes that correspond to different sets of underlying "knowledge-change processes". These modes of student engagement behavior are:

- *Passive engagement:* Learners receive information without additional mental or physical requirements (watching, listening, reading).

- *Active engagement:* Learners perform some type of physical action which focuses their attention on the material (e.g. underlining or highlighting text, rotating objects).
- *Constructive engagement:* Learners generate new information beyond what was provided in the learning materials (e.g. providing inferences, giving justifications, explaining in own words, creating a new drawing).
- *Interactive engagement:* Two people are partnered together conversing about the information, with both partners participating and the conversation focused on their constructive engagement with the material.

Student learning increases from Passive to Active to Constructive to Interactive activities [1]. The ICAP framework has been validated by a number of studies, including a successful study in an introductory materials science class [21], and can be used to guide the creation of more effective learning activities, including the activities in this paper.

The crystal structure activity presented in this paper is designed with two parts that engage students in the most effective *constructive* and *interactive* modes of the ICAP model. The individual portion of the activity is *constructive* because students synthesize information about atomic arrangements on planes, when only provided with the crystal structure in reduced sphere representation. They must construct and sketch the atoms of the given structure and plane using a space-filling representation of the atoms, thereby creating new knowledge that is not directly presented to them. The group activity is *interactive* because students converse in pairs or groups of three, first reviewing and critiquing the sketches they created individually. Then, the groups work together to generate the structure representations utilizing OVITO, with each individual sketching their work. The activities that the students talk about are, themselves, *constructive*.

2.2 Activity Description

The lesson is designed for a 50-minute introductory materials science course that covers crystal structures and atomic arrangements. The entire activity, including the student handouts, walk-throughs, program files, and the assessment instrument are available online at Ref. [22]. The activity consists of two parts. Part 1 is a constructive assessment on crystal structures, planes, and planar density, which students complete individually without referring to course materials. Part 2 consists of a small group activity where students use computers to visualize the planes and atomic arrangements to answer some of the same questions from Part 1.

The first two questions in Part 1 activate students' prior knowledge of Miller indices of common planes, and the names of the three cubic crystal structures that will be used in the subsequent activity (simple cubic (SC), FCC, and BCC). The planes are the (010), (110), and (111) planes, with no negative indices, so students may be able to answer this question by recall.

The third question presents students with a *constructive* activity. A drawing of the (010) plane in a cubic unit cell is presented alongside three drawings showing the FCC, SC, and BCC unit cells, all using the reduced-sphere representation of atoms, as shown in Figure 2. Students are asked to sketch the space-filling representation of the atoms lying on the given plane for each of the structures. The space-filling drawing of the atoms lying on the (010) plane in the FCC structure is provided as an example. After completing the set of three sketches, the students rank the planar densities of these three planes from highest to lowest. This is a constructive activity because students are *sketching* atoms on a plane using a *different perspective* than is provided, they are *changing representations* from reduced-sphere to space-filling representations of atoms, and they are *evaluating* the drawings to *rank* the relative planar densities.

3. For each crystal structure, draw a space-filling representation of the atoms that lie on the plane shown in the first column. Nearest-neighbor atoms should appear to touch as in the example. After completing the drawings, rank the planes from highest atomic density (1) to lowest (3).

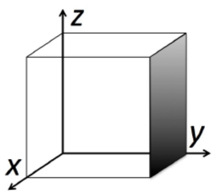
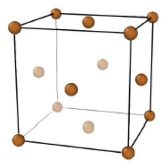
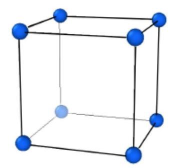
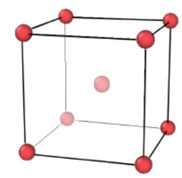
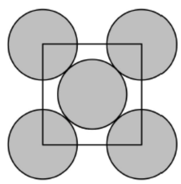
			
Space filling drawing of atoms lying on the plane shown.	 example		
Planar Density Rank (1 = highest)			

Figure 2. *Part 1, Question 3.* Students are asked to draw space-filling representations of atoms on the specified plane in three different structures, and then rank the three planes from highest to lowest atomic density.

By ranking the densities of the three planes, students engage with the content in a new way, adding to the constructive engagement in this portion of the activity. Students are not given an approach for this ranking, but are required to devise their own method, which could call upon them to derive meaning from the visualizations of the planes they sketched or involve them in numerical problem-solving to compare and contrast different planar arrangements of atoms to determine their relative densities, a *constructive* activity. This ranking activity is based on the unit cell ranking tasks in Ref. [23] and ranking tasks in physics education [24], without requiring students to explain their reasoning or certainty in the ranking.

Question 4 is constructed similarly to question 3, but instead of sketching and analyzing one plane in three different structures, students work with three different planes in one structure: the (110), (010), and (111) planes in the FCC structure, as shown in Figure 3.

4) Draw space-filling atomic planes for each plane shown in the FCC crystal structure, then rank the planes by planar density from highest (1) to lowest (3).

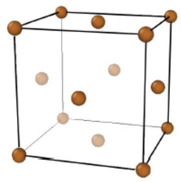
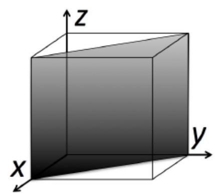
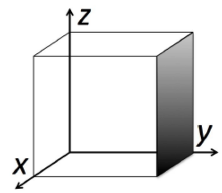
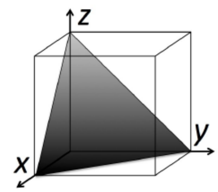
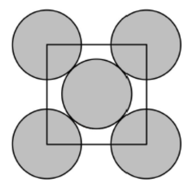
			
Miller Indices:			
Space filling drawing of atoms lying on the plane shown.		 example	
Planar Density Rank (1 = highest)			

Figure 3. *Part 1, Question 4.* Students draw space-filling representations of atoms on the specified planes for the FCC structure, and then rank the three planes from highest to lowest atomic density.

The 5th and final question in Part 1 asks students to identify the highest-density plane out of all of the sketches drawn in this part of the activity. This is intended to highlight the close-packed plane that is found in the FCC crystal structure.

Part 2 of the activity has students transition from individual work to working in groups of 2 or 3. In this part of the activity, students are introduced to OVITO, which they were instructed to install prior to class. Students are provided with step-by-step written instructions, accompanied by screenshots, in the *FCC Walkthrough* [22] for loading the FCC crystal structure into OVITO, and slicing the structure to display the (110) plane. Additionally, a spreadsheet is provided for calculating the distance from the origin to each of the planes. Students are provided with this geometric calculation to reduce cognitive load, allowing students to concentrate on learning to use OVITO for visualizing the desired crystal planes.

After sketching the planes utilizing OVITO, students evaluate their sketches from Part 1. They are instructed to note which drawings include the correct atoms on the planes, and whether the correct atoms touch. They are also asked to comment on errors in their individual work that were found using OVITO. This revision exercise is included because knowledge retention is increased when students identify their own misconceptions and errors [25].

The next portion of Part 2 asks students to investigate the NaCl structure, which also has an FCC Bravais lattice but with a two-particle motif. The *NaCl Walkthrough* leads students through an example for this activity, which includes viewing multiple unit cells.

Question 8 in Part 2 is intended to show students that the origin of a unit cell can be shifted and still result in the same structure; this question is as follows: "To help you see that either the Na^+ cation or the Cl^- anion could be drawn at the origin, repeat the NaCl unit cell to make a larger structure showing 2 x 2 x 2 unit cells. Draw the (010) plane of this larger structure in the box below. On your drawing, add two squares that outline two single unit cells, one with a Na^+ cation at the origin, and the other with a Cl^- anion at the origin."

Question 9 asks students to sketch space-filling representations of the (010), (110) and (111) planes in the NaCl structure, then rank the planar densities from highest to lowest, as shown in Figure 4.

9. Use Ovito to help you fill out the following table:

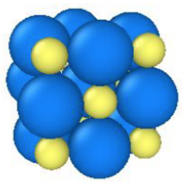
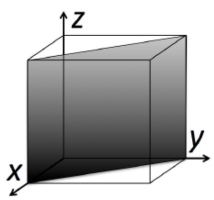
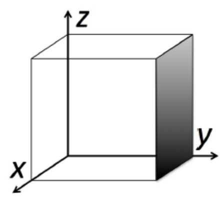
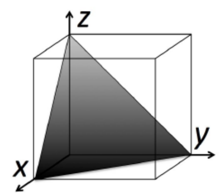
			
Miller Indices			
Distance			
Space-filling drawing of atoms lying on the plane shown.			
Planar Density Rank (1 = highest)			

Figure 4. *Part 2, Question 9.* Students are asked to draw space-filling representations of atoms on the specified planes for the NaCl structure, and then rank the three planes from highest to lowest atomic density.

The final question in Part 2 asks students to compare their drawings and planar density rankings for the (010), (110), and (111) planes in the FCC and NaCl crystal structures and write down the differences they identify.

Throughout Part 2, students are expected to work together and discuss and evaluate their sketches in order to rank the planar densities and find differences in the trends for different crystal structures. This active dialog between students engaged in constructive activities makes Part 2 an *interactive* activity.

2.3 Activity Implementation

The activity was implemented in an introductory materials science course offered across the engineering school at a large research institution. The course had three weekly lectures of 50 minutes each and one bi-weekly 1.5 hour lab, with an enrollment of 114 students. The activity was implemented during one of the regular lecture sessions.

The section of the course on crystal structures was comprised of six lectures followed by the in-lecture crystal structure activity. In the lectures, students were presented with information on crystal structures, identifying planes using Miller indices, and concepts of planar and linear densities, following the information commonly included in introductory materials science textbooks [26, 27].

In advance of the class, students were instructed to download OVITO onto their laptop computers, and bring their laptops to class. The computer-based activities were performed in groups, so students without a laptop or the software were instructed to find partners with working software.

The 50 minutes were used as follows: 15 minutes for the individual work (Part 1), 30 minutes for the group work (Part 2), and 5 minutes for a survey at the end. Students were given the worksheet for Part 1 at the beginning of class, and completed this individually. After the individual assessment, students kept their paper-and-pencil worksheets, and Part 2 of the activity was distributed to students. Students were instructed to begin Part 2 even if they did not complete Part 1. The student groups were encouraged to discuss their ideas as they worked together. During the final 5 minutes of class following the activity, students were requested to complete a voluntary survey about their perceptions of the activity.

2.4 Survey Design

The analysis of the pilot-test of this activity includes some preliminary assessment on the types of misconceptions exhibited by students, observations on the ease of implementation, and student feedback on the activity from a voluntary survey. The ten question survey (included in Ref. [22]) is adapted from the survey in Ref. [28], and investigates the ease of use of computational activities and perceived benefits of the activity. Questions 2-8 used a Likert-type scale. Select student responses are included anonymously, with the consent of the students.

3. Results and Discussion

3.1 Survey Responses on Student Perceptions and Attitudes

Students were surveyed on their perceptions of the lesson, and were asked to provide feedback on the lesson's ease of use, perceived effectiveness, and questions that arose as a result of the activity. 66 of the students in attendance submitted a survey. Appendix A contains the survey questions and results from 65 students; one survey contained very little information so was omitted from the results.

Students responded positively to the simulation activity, as 84% of students liked this type of visualization activity. More than half of students identified that these activities can be utilized in lectures or discussion sections, and a significant fraction felt the activities would be appropriate in homework or a lab. Only 2 students indicated that simulations should not be used at all. Furthermore, although this activity occurred in a large-lecture setting, the majority of students perceived the activity to be comparable or superior to laboratory exercises in terms of connection to the course (89% of students) and enhancing learning (91%). This possibly suggests that the visualization activity provides a venue for active authentic engagement with course material, similar to that of a laboratory class.

When designing simulation activities for a lecture, it is preferable to design them as *interactive*. This serves a dual purpose of accommodating students who are unable to install the software as well as enhancing the learning of all students. Students perceived benefits to working together, as 86% preferred working on a simulation with a partner; of these 56 students, 63% said that discussions should be encouraged. However, the nature of their discussions was not analyzed to determine the depth of conversations that occurred. The interactive mode requires students working together equally, discussing the *constructive* portion of the activity. Students' reflections could provide information on their discussions, but very few students responded to these questions on the survey. In the future, conversations should be monitored to ensure that they are constructive, possibly revising the discussion prompts as needed.

The low number of written responses for the reflection question may indicate that students were running out of time or uncomfortable with the nature of reflection in the learning process. This reflection question could be posed with more time, or at a later time online. Reflection on learning is a metacognitive activity that has been shown to improve student learning [25] so a revision of this activity will still include a reflection piece.

Faculty may be concerned that students will react unfavorably to installing and running simulation software on their own computers. However, 84% of students found that downloading the software and bringing their own computer was reasonable or very reasonable and easy to do; only 5 students responded negatively. This is similar to the results from Clark and Chamberlain [28] who found that students were not inconvenienced by running chemistry simulations on their personal computers. For the majority of the student population, the software installation poses no barrier to learning. Furthermore, performing the visualizations in groups mitigated the impact of technology problems that occurred in class.

The survey also provided feedback on the design of the activity. The activity's questions were at an appropriate level for students, as indicated by 84% of participants. 58% of students found the instructions to be adequate, but 37% wanted more specific instructions. It is unknown, however, whether students wanted more instructions on analysis in OVITO or drawing space-filling sketches of planes and ranking structures. Thus, it would be helpful to gather specific information on the areas where further instruction is needed.

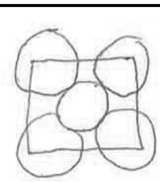
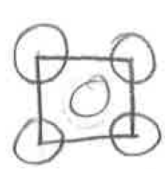
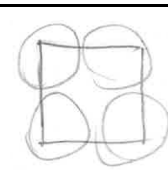
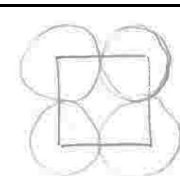
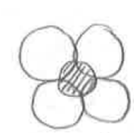
Logistically, the survey showed that the timing of the individual portion of the activity was appropriate, but Part 2 of the activity was too long. The average time to complete Part 1 was 11 ± 7 minutes, omitting the 11% of students who failed to complete the section. In contrast, 65% of students did not finish Part 2. These results indicate that 15 minutes is an adequate amount of time to complete Part 1, but Part 2 should be shortened to be completed in the allotted time.

3.2 Misconceptions Identified

The two-part crystal structure activity identified several misconceptions in students' understanding of atomic arrangement and planes. Samples of work from five students (identified here as students A, B, C, D, and E) are given in Tables 1-3, with results shown from both Parts 1 and 2. These students each show a variety of misconceptions about the atomic arrangements on the given planes. These misconceptions exist after learning the material formally in lecture, and can be compared to Krause and Waters' 2009 post-test results [2], which required students to sketch some of the same planar arrangements in crystal structures after receiving instruction on the topic.

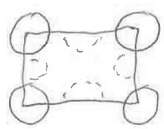
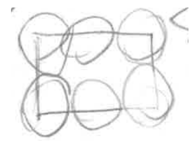
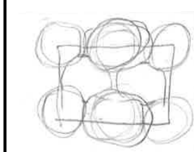
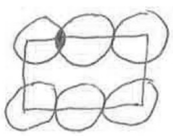
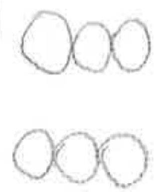
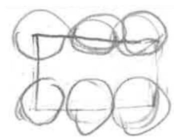
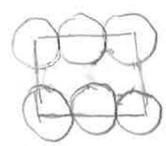
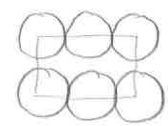
Part 1 elucidated several misconceptions in students' understanding of crystal structures. For the BCC (010) plane (Table 1), students A and B both erroneously included an atom in the center of the plane, whereas students C and D had the corner atoms touching. Student E showed both of these errors, with the corner atoms touching and an overlapping atom in the center. For comparison, Krause and Waters found that errors of extra atoms and atoms incorrectly touching occurred in 17% (combining the results for their answers B and C) and 24% of student responses, respectively [2].

Table 1. Student sketches of the BCC (010) plane, Part 1. The BCC (010) plane was not included in the Part 2 worksheet, so the results are only shown for Part 1.

Student Identifier	A	B	C	D	E
BCC (010) Part 1					

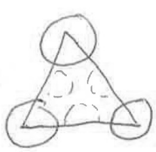
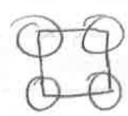
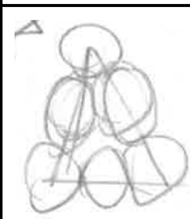
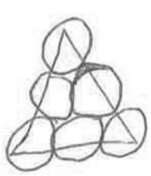
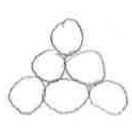
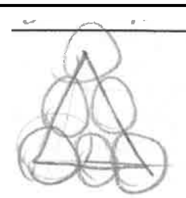
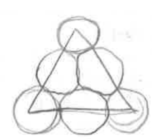
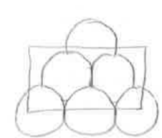
Students' sketches of the FCC planes also exhibited misconceptions in the atomic arrangement. For the (110) FCC plane, Krause and Waters identified the most common misconceptions as two answers in which the atoms were spaced incorrectly along the $[1\bar{1}0]$ direction. We noted a variety of incorrect answers in our student work. Table 2 shows that errors in the work of students A, B, and D include missing atoms along the $[1\bar{1}0]$ direction and extra atoms in the face. Student C was the only student to correctly place atoms along the $[1\bar{1}0]$ direction, but this student incorrectly spaced the atoms on the $[001]$ direction; this was noted in the student's comments at the conclusion of the activity.

Table 2. Student sketches of the FCC (110) plane taken from the worksheets for Parts 1 and 2.

Student Identifier	A	B	C	D	E
FCC (110) Part 1					?
FCC (110) Part 2					

Students consistently struggled with visualizing the FCC (111) plane; of the samples in Table 3, only student C was able to sketch the correct arrangement in Part 1. Student A is missing the atoms on the edges of the planes, while student B was unable to visualize the triangular geometry of the plane. Furthermore, student E was unsure about the atomic arrangement of this plane, and had the same problem with the FCC (110) plane.

Table 3. Student sketches the FCC (111) plane, taken from the worksheets for Parts 1 and 2.

Student Identifier	A	B	C	D	E
FCC (111) Part 1				[Blank]	?
FCC (111) Part 2					

The computer visualization activity significantly ameliorated student misconceptions. Of the five students whose work is shown here, all correctly sketched the atomic arrangements of the FCC (110) and (111) planes in Part 2. Notably, student E was initially unable to draw either of the FCC planes, but correctly drew these in Part 2. Furthermore, students' reflections during Part 2 indicate that they recognized their improvements. This was most obvious in the response of student D, who reported, "I couldn't really visualize where atoms in the (111) plane touched" when completing Part 1, and thus left the answer blank. However, this student successfully sketched both of the planes when visualizing these on the computer. Student C reported a similar comment, "Ovito helped me realize that the atoms in plane (110) do not touch from top to bottom". The preliminary qualitative analysis of this activity demonstrates that students can successfully identify errors in their prior sketches of atomic arrangements when visualizing the planes using OVITO.

3.3 Discussion of Activity Implementation and Suggested Changes

The activity is designed so that most students can successfully navigate the module with minimal support from the instructor, as directions for using the software are incorporated into the handouts. Students are requested to install the software prior to class, which most students were able to do without difficulty. The impact of any installation problems is alleviated by designing the computer activity for groups of two to three students, so that only one student per group needs to have the software installed. In the class studied, there was one group of two students who both had software installation problems. Neither student joined a different group, indicating that the instructor should be attentive to the dynamics in the room.

The activity is designed to work in one of the most common classroom environments: the large lecture hall. Large lecture classes typically have minimal flexibility, with a large number of students in fixed seating. The module format described in this paper (installation of OVITO on personal computers) allows a single instructor to run the activity in a lecture class of over 100 students. If resources are available, the activity could be conducted in a computer lab, where prior installation of the software would ensure that it is available for all students. The activity is also appropriate for a laboratory section, which could enhance opportunities for direct instructor support and feedback.

The student survey responses indicate that the activity handouts provided them with an appropriate amount of instruction, making this activity accessible to instructors with no prior OVITO expertise. Students had few in-class questions about the software, and most of those questions were answered in the handouts. A typical question was how to install the software. Other student questions related to the specifics of solving the problems, and did not require knowledge of the software. For example, some students requested direction in how to determine the planar densities (students were encouraged to develop their own methods). Another common question, also answered within the handouts, was the appropriate value for the distance from the origin to the plane.

This activity was generally successful, but revisions will be made based on findings from the pilot study. The interactive portion of the activity will be shortened by excluding the investigation of the NaCl crystal structure, which can be presented in a later assignment. This will allow students to focus on their learning gains and spend more time writing reflections on their uncovered misconceptions and new understanding.

Since all of the activity materials are provided online [22] along with an associated question and answer forum, feedback from other instructors who use the activity will be solicited and used to update the activity and online resources. The authors hope that materials science instructors from other institutions will share their experiences so that we can collaboratively gain insights into student learning and develop an optimized version of this activity.

4. Conclusions and Future Work

This work develops a new classroom activity that provides a visual and interactive method to deepen students' understanding about crystal structures. Students are introduced to a computer-based visualization tool used by materials science researchers. This activity is successfully implemented in a large class environment with very little instructor support.

This initial study indicates the module is effective at correcting some of students' prior misconceptions about crystal structures, while students also perceive a benefit from participation. At the beginning of the activity, students' sketches show many of the errors previously identified by Krause and Waters [2]. Some of these errors are then corrected when completing the module. However, the significance of the learning gains was not quantified.

We plan to study the effect of the module on student learning gains, as well as the persistence of these gains over the course of the semester. The Crystal Structure Visualization Survey [2] can be utilized to easily measure the effectiveness of the interactive activity (and supporting or alternative activities) in an instructor's class. These analyses can be performed in a single classroom or over multiple classes across universities, with input from additional instructors.

Acknowledgements

This work was made possible in part by a grant from the National Science Foundation (EEC 1227110). Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation.

Some of the data analysis and representation was performed using Igor Pro (WaveMetrics, Inc., Oregon, USA) https://www.wavemetrics.com

References

[1] Chi, M.T.H. and R. Wylie, *The ICAP Framework: Linking Cognitive Engagement to Active Learning Outcomes.* Educational Psychologist, 2014. **49**(4): p. 219-243.

[2] Krause, S. and C. Waters, *Uncovering and Repairing Crystal Structure Misconceptions in an Introductory Materials Engineering Class*, in *2012 Frontiers in Education Conference Proceedings*. p. 1-6. 2012.

[3] Ohashi, A., *Using Latex Balls and Acrylic Resin Plates To Investigate the Stacking Arrangement and Packing Efficiency of Metal Crystals.* Journal of Chemical Education, 2015. **92**(3): p. 512-516.
[4] Collins, D.C., *A Unit Cell Laboratory Experiment: Marbles, Magnets, and Stacking Arrangements.* Journal of Chemical Education, 2011. **88**(9): p. 1318-1322.
[5] Cushman, C.V. and M.R. Linford, *Using the Plan View To Teach Basic Crystallography in General Chemistry.* Journal of Chemical Education, 2015. **92**(8): p. 1415-1418.
[6] Foley, B., *Using Visualization Tools to Improve Undergraduates' Understanding of Crystal Structure*, in *1996 Frontiers in Education Conference*. p. 1079-1083. 1996.
[7] *CrystalMaker Software: Crystal and Molecular Structures Modelling and Diffraction*. [Accessed 2/1/2017]; Available from: http://www.crystalmaker.com/.
[8] Luealamai, S. and B. Panijpan, *Learning About the Unit Cell and Crystal Lattice With Computerized Simulations and Games.* Simulation & Gaming, 2012. **43**(1): p. 67-84.
[9] *Materials Genome Initiative for Global Competitiveness*. 2011, National Science and Technology Council.
[10] Thornton, K., et al., *Computational Materials Science and Engineering Education: A Survey of Trends and Needs.* JOM, 2009. **61**(10): p. 12-17.
[11] *A Report of the National Science Foundation Advisory Committee for Cyberinfrastructure*. 2011, National Science Foundation.
[12] *Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security*. 2008, National Research Council: Washington, DC. p. 152.
[13] *Modeling Across Scales: A Roadmapping Study for Connecting Materials Models and Simulations Across Length and Time Scales*. 2015, The Minerals, Metals, Materials, Society: Warrendale, PA.
[14] Li, L., *Integrating Computational Modeling Modules into Undergraduate Materials Science and Engineering Education*, in *American Society for Engineering Education Annual Conference*. p. 14441. 2016.
[15] Magana, A.J., M.L. Falk, and M.J. Reese Jr., *Introducing Discipline-Based Computing in Undergraduate Engineering Education.* ACM Transactions on Computing Education, 2013. **13**(4): p. 1-22.
[16] Mansbach, R., et al., *Reforming an Undergraduate Materials Science Curriculum with Computational Modules.* Journal of Materials Education, 2016. **38**: p. 161-174.
[17] *OVITO Open Visualization Tool*. [Accessed 1/16/2017]; Available from: http://www.ovito.org/.
[18] Stukowski, A., *Visualization and Analysis of Atomistic Simulation Data with OVITO–The Open Visualization Tool.* Modelling and Simulation in Materials Science and Engineering, 2009. **18**(1): p. 015012.
[19] *Google Scholar: Visualization and Analysis of Atomistic Simulation Data with OVITO–The Open Visualization Tool*. [Accessed 2/3/2017]; Available from: https://scholar.google.com/scholar?cluster=17004772467538201275&hl=en&as_sdt=800005&sciodt=1,15.
[20] Freeman, S., et al., *Active Learning Increases Student Performance in Science, Engineering, and Mathematics.* Proceedings of the National Academy of Sciences, 2014. **111**(23): p. 8410-8415.

[21] Menekse, M., et al., *Differentiated Overt Learning Activities for Effective Instruction in Engineering Classrooms.* Journal of Engineering Education, 2013. **102**(3): p. 346-374.
[22] Gentry, S. and T. Faltens, *Visualizing Crystal Structures: An Interactive Group Classroom Activity.* 2016 [Accessed 1/18/2017]; Available from: https://nanohub.org/resources/25263.
[23] Faltens, T., *Unit Cell Ranking Tasks, from nanoHUB*. 2012 [Accessed 2/1/2017]; Available from: https://nanohub.org/resources/15427.
[24] *Ranking Task Exercises in Physics*. [Accessed 2/1/2017]; Available from: https://www.physport.org/methods/method.cfm?G=Ranking_Tasks
[25] Brown, P.C., H.L. Roediger III, and M.A. McDaniel, *Make It Stick: The Science of Successful Learning*. 2014, Cambridge, MA: Belknap Press.
[26] Callister, W.D. and D.G. Rethwisch, *Materials Science and Engineering: An Introduction*. 9th ed. 2014, Hoboken, NJ: John Wiley and Sons.
[27] Shackelford, J.F., *Introduction to Materials Science for Engineers*. 8th ed. 2015, Boston, MA: Pearson.
[28] Clark, T.M. and J.M. Chamberlain, *Use of a PhET Interactive Simulation in General Chemistry Laboratory: Models of the Hydrogen Atom.* Journal of Chemical Education, 2014. **91**(8): p. 1198-1202.

Appendix A: Survey Questions and Fall 2016 Survey Response Data

<u>Atomic Structures Post-Activity Survey</u>

1. How long did each activity take?

a. ______ minutes for Individual activity or _____ did not finish in allotted time

b. ______ minutes for Ovito activity or _____ did not finish in allotted time

54 students responded with times for the individual and group activities, with the results displayed in Figure 5. For the students who completed the individual activity, the average time reported was 11±7 minutes. 7 students did not complete the individual activity. Of the students that finished the group activity, the average time to complete this section was 24±10 min. 42 students did not complete the group activity.

For both the individual and group activities, students who did not complete the activity were assigned a time of 60 minutes so that their data appears in the histograms for visual comparison. This bar is marked DNF (Did Not Finish) on each histogram.

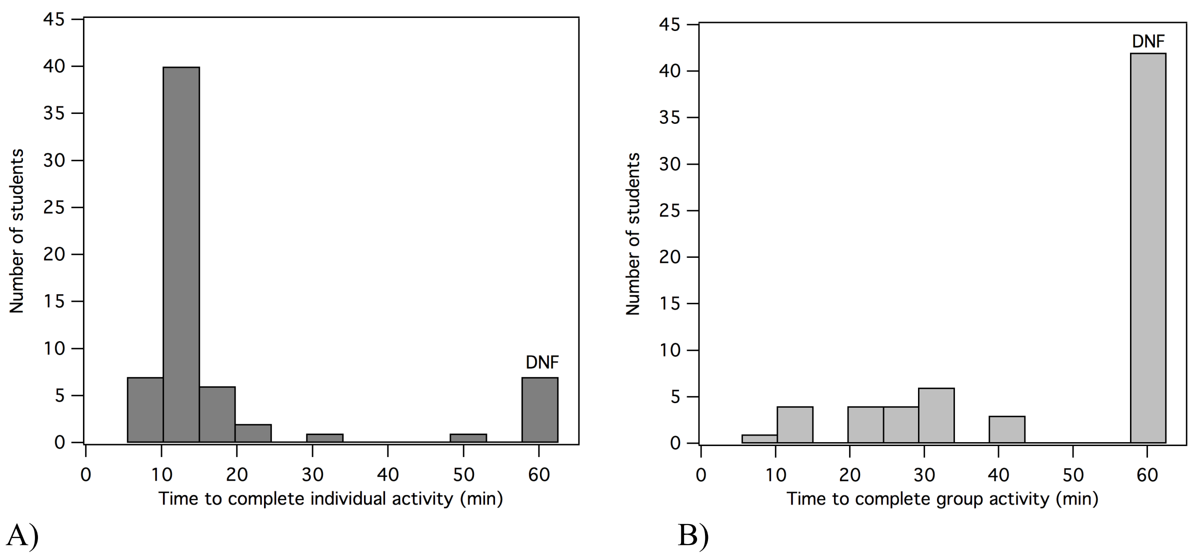


Figure 5. Histograms showing the A) time for students to complete Part 1 and B) time for students to complete Part 2 of the activity. Students who did not complete the part of the activity were assigned a time of 60 minutes and appear as the DNF (Did Not Finish) bar in each histogram.

For questions 2-9, check the box below the statement to indicate the response you most agree with.

The percentage of students responding to each option is indicated, with the number of students following in parentheses. The first and next most popular responses are highlighted in medium grey and light grey, respectively.

2. How enjoyable are class activities that include simulations/visualizations?

Strongly dislike	*Somewhat dislike*	*Neutral*	*Somewhat like*	*Strongly like*
2% (1)	3% (2)	12% (8)	**46% (30)**	38% (24)

3. Downloading the software and bringing a computer to lecture was…

Very difficult	*Somewhat unreasonable*	*No opinion*	*Somewhat reasonable*	*Very reasonable, easy to do*
6% (4)	1% (1)	8% (5)	**48% (31)**	36% (23)

4. It is better to work on a simulation…

Alone, group discussions discouraged	*No guidelines provided*	*Alone*	*With a partner*	*With a partner, discussions encouraged*
2% (1)	(0)	11% (7)	33% (21)	**55% (35)**

5. The activity should have had…

Fewer instructions	*Somewhat fewer instructions*	*About the same*	*Somewhat more specific instructions*	*Step-by-step instructions*
(0)	5% (3)	**58% (38)**	20% (13)	17% (11)

6. The questions in the activity were…

Too easy, "busy work"	*A little too easy*	*About right*	*A little too difficult*	*Far too difficult*
2% (1)	9% (6)	**84% (54)**	5% (3)	(0)

7. Compared to Lab 1 in this class, this activity was...

Not connected to class	*Less connected*	*About the same*	*More closely connected*	*Very connected*
(0)	9% (6)	33% (21)	**41% (26)**	17% (11)

8. Compared to other labs (Lab 1 in this class and labs in other classes, such as chemistry), my learning was...

Much less than normal	*Somewhat less*	*About the same*	*Somewhat more*	*Much more*
2% (1)	5% (3)	32% (20)	**43% (27)**	19% (12)

9. Simulations should be used: (check all that apply)

_____ *as homework*	46% (30)
_____ *in a discussion section*	65% (42)
_____ *in lab*	29% (19)
_____ *in lecture*	**74% (48)**
_____ *not used*	3% (2)

10. Student reflections
a) What did you find most interesting or eye-opening about this activity?

b) Generate at least 2 questions you have about structures of materials or how we visualize or work with them.