Integrating a Research-Grade Simulation Tool in a Second-Year Materials Science Laboratory Course

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Abstract

Students have difficulty conceptualizing phenomena that are not directly visible. For example, students struggle to understand the atomic-level processes responsible for plastic deformation in metals. This paper reports on an innovative laboratory lesson redesign that better integrates the simulation and traditional tensile test components of a unit on plastic deformation that is completed by second-year Materials Science and Engineering students. This paper will discuss the evolution of the unit and present findings from the most recent end-of-semester exam as evidence of progress in developing an integrated laboratory experience that supports student learning of these concepts. Current thinking concerning the laboratory design is shared.

Introduction

Previous work has shown that concepts related to the deformation of metals are difficult for many engineering students to learn. Students may struggle with remembering the proper definitions for new terminology used to describe the features of engineering stress vs. strain curves, with understanding features of the macroscopic behavior of metals observed in the elastic vs. plastic regions, and in relating the physical properties and behavior of metal samples with the way this behavior is portrayed in stress-strain curves[1]. Furthermore, students struggle to understand the "invisible" atomic-level processes of dislocation formation and dislocation motion that control plastic deformation[2,3], and how these relate to the sample geometry and externally applied forces that drive the deformation. Some researchers have used specially designed group worksheets[1] and concept sketching[4] to engage students at a higher level with these concepts.

Another way for students to actively construct knowledge about the atomic-level processes involved in the deformation of metals is by interacting with simulations that allow them to view the behavior of discrete atoms in previously invisible processes. Simulation tools built on realistic physical models are available at no cost on nanoHUB.org[5] and allow students to virtually experiment at the atomic-level. The nanoHUB simulation tools are run on remote servers via a web browser, so they do not require any local computing resources or software installation, and they are thus easily accessible in a classroom environment. Integrating simulation tools into the classroom is supported by recommendations from the National Research Council (2000) report, *How People Learn*, which endorses the integration of technology with curricular materials to support student learning[6].

Despite the appeal of the effect that simulations could have on student learning, previous research on the inclusion of interactive simulations that allow students to test materials at the atomic level in a materials science laboratory course was not able to demonstrate the effectiveness of the simulation lab in creating a deeper student understanding of dislocation motion and slip[7]. This is consistent with the observation that the mere inclusion of technology in the classroom may not be sufficient to enhance student learning[6].

Our own experience over several terms with a metallic deformation lab that incorporates atomic-level simulations is that even with the addition of simulation-based activities, students continue to struggle to explain the atomic-level processes responsible for metallic deformation[8]. A brief history of the development of this lab follows.

In 2009, a 3-hour stand-alone simulation laboratory using molecular dynamics (MD) simulations was created. This lab had four learning objectives: (1) Develop an atomic picture of plastic deformation in metals, (2) Understand the orientation of the active slip system with respect to the tensile axis, (3) Estimate the strength of perfect crystals and compare it to polycrystalline samples, and (4) Explore strain hardening focusing on the difference between annealed and cold worked macroscopic samples and nanoscale samples[9].

This lab was piloted at the end of *MSE 235 - Materials Laboratory*, at Purdue University in Fall 2009. Limited results from a 4-item pre-post assessment indicated that students had an "increased conceptual understanding of how the atomic structure of a material changes under various conditions", and it was surmised that visualization of the atomic behavior enabled deeper learning of the concepts[7].

Building on the results of this trial, in Fall 2013 the simulation laboratory was combined with a traditional mechanical tensile testing of metals laboratory to enable students to make direct comparisons of nanoscale and macroscale results. In Summer 2014, *MSE 235* students' work, consisting of in-lab worksheets, lab reports, and exam questions, was collected and examined for their understanding of nanoscale and macroscale deformation of metals[10]. Findings similar to the 2009 trial were not evident in the combined laboratory exercise; students struggled to articulate the atomic-level processes occurring when different materials are under strain. Reasons for the unreplicable findings may lie in: (1) the placement of this lab within the semester, (2) changes in the instructional team resulting in different pedagogical approaches, (3) characteristics of the off-semester student population, and (4) different evidence of student learning of the concepts (pre-post assessment versus student work products)[8].

Work on the integration of the MD simulations with the traditional tensile test laboratory has continued[11], and is focused on improving the entire learning package and better understanding the nature of the struggles students have with understanding the processes fundamental to the atomic mechanisms of metallic deformation. A framework based on best practices in education has been created for effectively incorporating simulations into lessons[12]. Following this framework, the laboratory learning objectives have been reevaluated and updated and refinements made to the pre-lab and in-class lab exercises, laboratory reports, and associated exam questions[13]. The updated learning objectives for the laboratory are listed in Table 1.

Table 1: Learning Objective for the Fall 2015 Tensile Test Laboratory

Learning Objectives	
1	Explain the experimental steps required to perform a valid tensile test.
2	Graph stress-strain curves given force vs. elongation (or time) data for a tensile test.
3	Determine the characteristic features of stress-strain curves (i.e., elastic region, plastic region, Young's modulus (E), yield strength (σ_y), ultimate tensile strength (UTS)).
4	Explain plastic deformation at the atomic level in terms of dislocation motion and slip.
5	Apply your knowledge of crystallography to describe, using Miller Indices, the active slip systems in FCC metals.
6	Differentiate plastic deformation for macro-versus nano-sized metals. Explain reasons for similarities in the Young's modulus and differences in yield strength between *defect free nanoscale* single crystals and *macroscale* polycrystalline samples.

The purpose of this paper is to assess effectiveness of the refined hybrid tensile testing laboratory on student's learning of the atomic-level mechanisms associated with deformation of metals.

Methods

Participants and Setting

The setting for this study was the Fall 2015 offering of a required sophomore-level materials engineering course at Purdue University. *MSE 235: Materials Laboratory* introduces students to the relationship between the structure and properties of materials through both lecture and laboratory sessions. Lectures are used to introduce students to the relevant concepts before each laboratory session and to debrief them afterwards. *MSE 235* is the first materials laboratory course and trains students in the use of basic "tools of the trade" that they will use and build upon in subsequent materials engineering courses. Students in this course have either already taken or are concurrently enrolled in *MSE 230: Structure and Properties of Materials*. *MSE 230* is an introductory materials science course detailing the structure, properties, and processing of engineering materials, including the relationships between the different levels of internal structure and basic properties, as well as ways material structures (and thus properties) are controlled and manipulated in basic processing operations. Fifty students were enrolled in *MSE 235* in Fall 2015; 48 students took the final exam (one student dropped the course while another never attended a single lecture).

Tensile Test Lab

The goal of integrating nanowire simulations with the tensile testing laboratory is to help students understand and visualize the atomic-level mechanisms associated with plastic deformation. By presenting these together, students may build an intuitive feel for how plastic deformation is linked across length scales as they first learn these concepts. The unit of instruction for the laboratory consists of multiple parts. A pre-lab lecture introduces stress-strain curves, characteristic measurements, and atomic-level processes. Students read the laboratory instructions prior to the lab and answer pre-lab questions about the mechanical test. During the lab, students perform mechanical testing of ductile metal samples and generate stress-strain curves. Students also run MD simulations to perform virtual tensile testing of copper nanowires. These simulations generate a stress-strain curve along with visualizations of the structural changes that occur throughout the test.

Interweaving the two sets of lab activities reduces the time students spend waiting for equipment and allows them more time for hands-on activities and active engagement with the material. During the lab, students work in small groups as they perform the experimental procedures, collect and share data, and discuss and respond to a set of questions on a group worksheet. They prepare a group lab report and also submit individual detailed answers to several conceptual questions related to the lab.

The MD simulations are performed using the *Nanomaterial Mechanics Explorer*, an online application provided by nanoHUB.org[14] that is powered by the open-source *LAMMPS* Molecular Dynamics Simulator[15] and that was created to complement this hybrid lab, keeping the novice student user in mind. This tool provides a simple and intuitive graphical interface for students to explore mechanical properties of materials. Compared to the previously used nanowire tensile testing tool on nanoHUB[16], the new tool simplifies the default user interface and reduces the amount of input required from the user to run a simulation. For example, in the previous tool students needed to create and enter a programing script to construct nanowires with different crystallographic orientations. In the new tool, the default settings allow students to easily select a pre-made nanowire aligned along the [100], [110], or [111] directions. Output from the MD simulation includes a series of interactive visualizations of the atoms in the nanowire that are captured at various times throughout the process along with the associated stress-strain curve, as shown in Figure 1. The simplified interface in the new simulation tool has an “Advanced” option that allows students to access all of the simulation input variables in order to change features such as the nanowire size, shape, strain rate, or temperature for further investigation.

During the lab period, the class is split in half, one set of students starts with the traditional tensile tests on copper and brass specimens, and the other starts with the simulation activities. Learning Objectives 1 to 3 (Table 1) are addressed in the traditional tensile testing portion of the laboratory. Students work in groups of about 4 and use two tensile frames to generate complete stress-strain curves for sets of copper and brass samples. They learn to use an extensometer to record strain so that accurate values of Young’s modulus can be calculated.

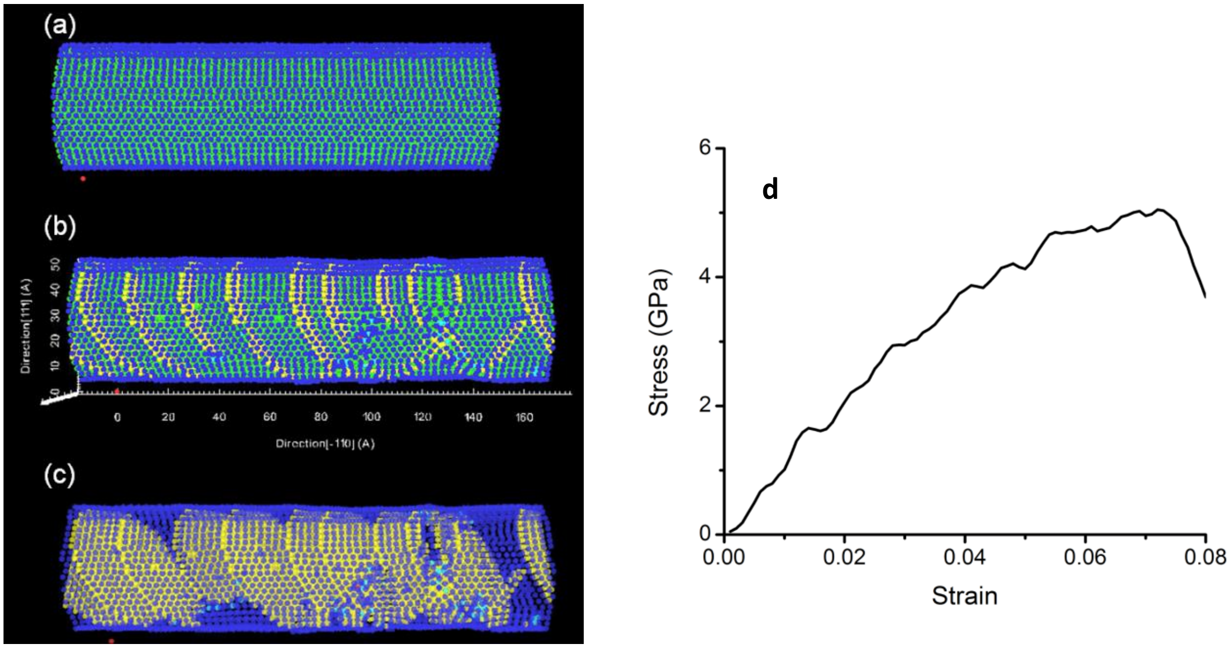
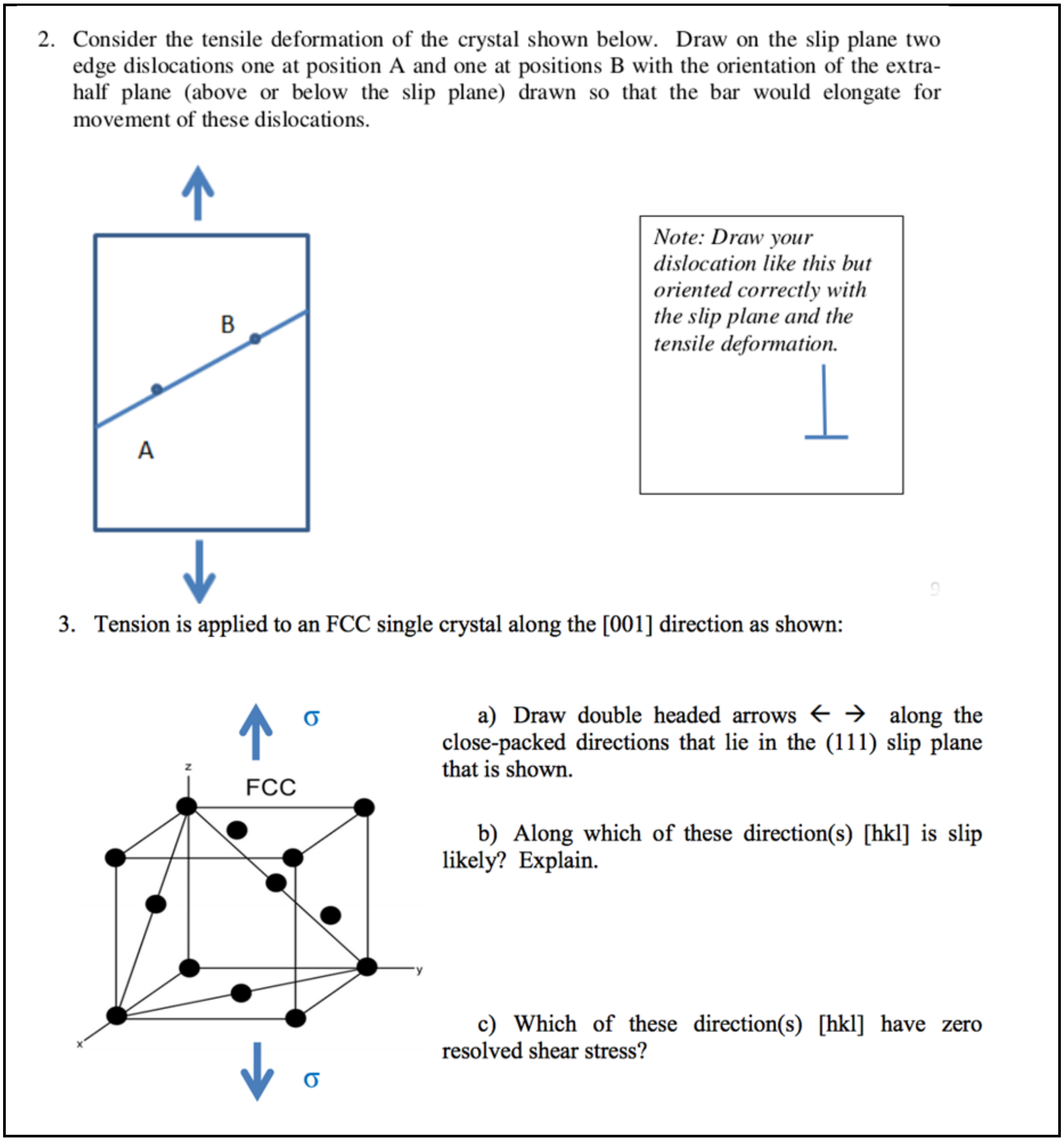


Figure 1: Images of a <110> oriented Cu nanowire in which slip occurs via a/6<112> Shockley partial dislocations, resulting in a non-FCC atomic coordination for atoms around the slip plane, which are shown in yellow. Atoms with FCC coordination are shown in light blue and surface atoms are dark blue. 1(a) is the initial unloaded and defect-free single crystal. 1(b) is the nanowire just after yielding, and shows evidence of slip. 1(c) is the "defect view", which shows only the atoms that have non-FCC coordination. 1(d) is the corresponding stress-strain curve. A detailed description of these images is given by Coughlin[11].

Learning Objectives 4 and 5 (Table 1) are addressed in the simulation portion of the laboratory. The student groups answer worksheet questions that require them to individually run simulations of nanowires with different orientations. While the simulations run, the student groups discuss concepts related to dislocation line defects, the relationships between dislocation glide and crystalline slip, and the meaning of *resolved shear stress*. The student groups are also asked to predict the active slip planes for [100], [110], and [111] oriented FCC crystals and to compare their predictions with the simulation results. Examples of the questions that the students discuss are shown in Figures 2 and 3.

These questions are given to the students in the form of a worksheet to be completed during the laboratory period. The students keep their individual completed worksheets for future reference and submit a group lab report six days after the lab session. Working in groups to complete the majority of the lab submission encourages students to communicate with their peers and also allows them to complete the report in a reasonable amount of time.



2. Consider the tensile deformation of the crystal shown below. Draw on the slip plane two edge dislocations one at position A and one at positions B with the orientation of the extra-half plane (above or below the slip plane) drawn so that the bar would elongate for movement of these dislocations.

Note: Draw your dislocation like this but oriented correctly with the slip plane and the tensile deformation.

3. Tension is applied to an FCC single crystal along the [001] direction as shown:

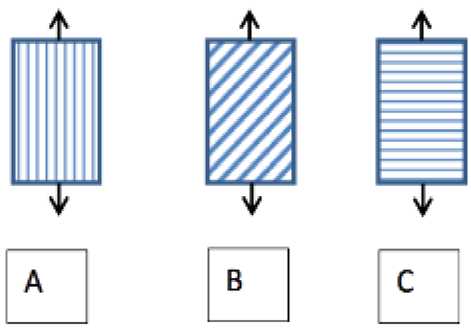
a) Draw double headed arrows ← → along the close-packed directions that lie in the (111) slip plane that is shown.

b) Along which of these direction(s) [hkl] is slip likely? Explain.

c) Which of these direction(s) [hkl] have zero resolved shear stress?

Figure 2: An example of one of the discussion questions related to Learning Objective 4 that the students answer while working in small groups.

4. Consider a tensile sample and three different sets of planes (shown below). For the <u>same</u> applied normal stress, which set of planes experiences the highest shear stress (circle it)? Explain your answer.



5. Now consider testing your nanowire along different crystallographic directions as listed below. For the four possible {111} slip planes, on which does slip actually occur. To show this, use the notation in Problem 4 to highlight this.

Testing axis [100] -- slip plane best corresponds to what condition above A, B or C

$(1\,1\,1)$ ________

$(\bar{1}\,1\,1)$ ________

$(1\,\bar{1}\,1)$ ________

$(\bar{1}\,\bar{1}\,1)$ ________

How many different sets of slip planes are observed from the simulation?

Your Answer:________________

Figure 3: An example of one of the discussion questions related to Learning Objective 5. Students are also asked to consider the [110] and [111] testing orientations (not shown).

To further encourage post-lab reflection on the results and to address Learning Objective 6, students are also required to submit individual assignments the week after the lab session. In these reports, students are asked to discuss the results from both the standard tensile tests and nanowire simulations and to complete a simple problem related to calculating the Schmid factor for FCC slip. Specifically, the following questions are asked:

1. How does the yield stress of a copper nanowire compare to the yield stress of copper sample? Why is there a difference or similarity in strength? Hint: refer to your group worksheet.

2. How does the Young's modulus of a copper nanowire compare to that of the macroscale copper sample? Why is there a difference or similarity in Young's modulus? Hint: refer to your group worksheet.

3. Compare your results from questions 1&2 with the values for copper listed in your textbook.

4. Consider a large single crystal of copper (10 nm diameter) oriented such that a tensile stress is applied along a [001] direction. If slip occurs on a (111) plane in a $[\bar{1}01]$ and is initiated at an applied tensile stress of 12 MPa, compute the critical resolved shear stress.

5. Generate at least two questions that you have about the MD simulations output with regards to understanding plastic deformation at the atom scale for macro- and nano-sized specimens.

Student responses to question 1 of the individual report were previously analyzed and reported[11].

Data Collection & Analysis

In this work, students' responses to four multiple choice questions on the final exam were evaluated for evidence of their understanding of the atomic-level processes responsible for deformation in metals. Each question aligns with one of the laboratory's learning objectives, and is asked in two parts. In the first part, the students are asked to select the best response to complete a statement. In the second part, the students are asked to select a rationale to support their complete statement in part one.

Results

The first two final exam questions focused on the concepts of *Young's modulus of elasticity* and *yield strength*. Students were asked to compare the relative magnitudes of these quantities for macroscopic polycrystalline copper samples and for nanowire copper samples. The questions were presented in a two-part format, where in the first part students indicated *what* the relationship is, and in the second part the *reason* for this relationship.

The relationships and underlying reasons were covered in the lab, and students previously answered two similar open-ended questions in their individual lab reports. Some of the ideas for the *reason* distractors were taken from the students' lab reports, and the overall set of distractors for a given question was designed to contain more than one possible reason for each of the three potential answers for the first part. In other words, there is more than one reason that would make something about the nanowire *similar to, smaller than,* or *greater than* the macroscopic sample.

The first question focused on Young's Modulus of elasticity. Students previously addressed the concepts in this question in both their group and individual lab reports. In the group reports, they calculated Young's modulus for copper using raw data from their tensile tests and compared this value to that obtained from the nanowire simulation and to values from the reference literature. The two-part exam question was stated as:

1) Compared to a macroscopic polycrystalline copper tensile sample, a copper nanowire sample will have a **Young's Modulus** that is:

(a) higher
(b) similar
(c) lower

Because the nanowire:

(i.) has a smaller cross sectional area
(ii.) is a single crystal
(iii.) has the same orientation
(iv.) is made of the same material
(v.) has no preexisting dislocations
(vi.) has a similar dislocation density
(vii.) has a greater dislocation density
(viii.) has greater interatomic bonding forces

The student responses to this question are presented in Table 2. Of the 48 students who took the final exam, one student did not answer question 1 in a way that could be interpreted; this student's response was not included in this analysis. Only 46.8% of the remaining 47 students selected the correct response (b iv). All students who selected an answer stating that the macroscopic and nanowire samples have a similar (b) Young's Modulus also indicated an understanding that this is because the Young's Modulus is a materials property (iv).

Table 2. Number of student responses to exam question 1.

Response	i	ii	iii	iv	v	vi	vii	viii	multiple	Total
a	3	5	-	4	4	-	-	1	4	21
b	-	-	-	22	-	-	-	-	-	22
c	-	-	-		3	-	-	-	1	4
Total	3	5	-	26	7	-	-	1	5	47

Those that selected that the nanowire has a higher (a) or lower (c) Young's Modulus compared to the macroscopic sample focused on characteristics that describe the nanowire. The nanowire does have a smaller cross-sectional area (i), is a single crystal (ii), and has no preexisting dislocations (v). All these characteristics were highlighted in the lecture and laboratory discussions, and thus some students may have just selected terms that they recognized. The incorrect selections may also indicate an incomplete understanding of the definitions of stress versus force, the differences between elastic and plastic deformation, or the shape of the tensile stress-strain curve.

The five students that circled multiple reasons for their selection of higher or lower Young's Modulus also tended to focus on characteristics that describe the nanowire (i, ii). Two included in their responses that the nanowire has a similar dislocation density (vi). Three of these students included the fact the Young's Modulus is a materials property (iv).

The second question focused on yield stress, and contains the same selections and distractors as the first question:

2) Compared to a macroscopic polycrystalline copper tensile sample, a copper nanowire sample will have a **yield stress** that is:

(a) higher
(b) similar
(c) lower

Because the nanowire:
(i.) has a smaller cross sectional area
(ii.) is a single crystal
(iii.) has the same orientation
(iv.) is made of the same material
(v.) has no preexisting dislocations
(vi.) has a similar dislocation density
(vii.) has a greater dislocation density
(viii.) has greater interatomic bonding forces

The student responses to this question are presented in Table 3. Here again, one student did not answer question 2 in a way that could be interpreted; this student's response was not included in this analysis. While 85.1% of the students selected that the yield stress of the nanowire sample would be greater (a) than the macroscopic sample, only 31.9% of those students correctly attributed the difference to the lack of preexisting dislocations (v). The remaining students selected reasons that involve characteristics that describe the nanowire (i, ii, vii).

Table 3. Number of student responses to exam question 2.

Response	i	ii	iii	iv	v	vi	vii	viii	multiple	Total
a	8	10	-	-	15	-	1	-	6	40
b	1	-	-	-	-	-	-	-	-	1
c	-	1	-	-	4	-	-	-	1	1
Total	9	11	-	-	19	-	1	-	7	47

While eighteen students (32.3%) were able to correctly complete the statements in the first part of both questions 1 and 2, only six students (12.7%) were able to provide the correct reasons for both statements.

The second two final exam questions focused on the concept that plastic deformation is driven by shear stresses. The students had previously discussed the concepts that slip and dislocation motion are driven by shear stresses in their group discussions, and they performed a Schmid's Law calculation in their individual report. The two exam questions were very similar to examples that the students previously worked with in problem 5 of the group lab worksheet, as shown in Figure 3.

Question 3 presents a situation where slip *is* possible:

3) A copper single crystal is tested in tension along the [110] direction. **The (111) plane:**

(a) is a possible slip plane
(b) is not a possible slip plane

Because the plane:
(i.) is parallel to the tensile axis
(ii.) is inclined to the tensile axis
(iii.) is perpendicular to the tensile axis

The corresponding student responses are presented in Table 4. For this question, 68.8% responded with the correct answer (a ii).

Table 4. Number of student responses to exam question 3.

Response	i	ii	iii	Total
a	2	33	3	39
b	1	7	2	9
Total	3	40	5	48

Question 4 presents a case where the resolved shear stress is zero and slip is not possible:

4) A copper single crystal is tested in tension along the [110] direction. **The** $(\bar{1}\,1\,1)$ **plane**:

(a) is a possible slip plane
(b) is not a possible slip plane

Because the plane:
(i.) is parallel to the tensile axis
(ii.) is inclined to the tensile axis
(iii.) is perpendicular to the tensile axis

For this question, only 32.1% of the students responded with the correct answer (b i), as listed in Table 5.

Table 5. Number of student responses to exam question 4.

Response	i	ii	iii	Total
a	6	3	8	17
b	15	2	14	31
Total	21	5	22	48

Considering the two questions together, thirty students (62.5%) were able to select the correct starting statements for both questions 3 and 4. However, only twelve students (25.0%) were able to provide the correct reasons for both statements.

There are 3 logically consistent response pairs possible for questions 3 and 4: (a ii) for the case where slip is possible for the plane and direction given, and (b i) or (b iii) for the case where slip is not possible because the resolved shear stress is zero. For question 3, 36 students (75%) selected consistent response pairs with 92% of these being the correct answer. For question 4, by contrast, 32 students (67%) selected consistent response pairs, but only 47% of these were correct.

Although students were not required to show their work or defend their answers for these exam questions, many made a sketch, calculated a dot product, or did both for questions 3 and 4. There is an interesting correlation between student responses and the methods they employed. In the following, only the work shown is discussed, and it is understood that some students may have mentally done work without writing anything on the page.

For question 3, 27 students attempted a sketch, and of these, 19 (70%) were clearly correct. For question 4, 22 students attempted a sketch, but only 9 (41%) of these were clearly correct. It is likely that the negative index in the plane in question 4 made sketching more difficult for the students.

The 17 (89%) students with correct sketches for problem 3 answered the problem correctly. While all 9 of the students with correct sketches for problem 4 correctly indicated that the plane was parallel to the tensile axis, only 5 of these students (56%) selected the correct answer pair. Thus these students are having trouble comprehending the meaning or implications of a resolved shear stress.

In both questions 3 and 4, all students who attempted a dot product calculated the dot product correctly. For question 3, 8 students attempted a dot product; of these, 6 (75%) answered the problem correctly. Two of these 6 also drew sketches. For question 4, 5 students showed work for a dot product; of these, only 1 (20%) answered the problem correctly, and this student also drew a correct sketch. Significantly, no students who only showed work for a dot product, but not a sketch, answered this problem correctly.

It seems likely that students took the dot-product between the tensile direction [$\mathbf{1\ 1\ 0}$] and [$\mathbf{\bar{1}\ 1\ 1}$] and noted an orthogonal relationship without remembering that the [$\mathbf{\bar{1}\ 1\ 1}$] direction is itself orthogonal to the ($\mathbf{\bar{1}\ 1\ 1}$) plane. Since the dot product is fairly easy to compute, more students likely did a mental calculation without writing down any work. Computing a dot product for a non-orthogonal pair of directions would yield a correctly interpreted answer, which may be another reason why more students answered question 3 correctly than question 4.

Overall, of the methods used, sketching yielded a higher percentage of correct answers than computing a dot-product (or showing no work), and students who showed work with both sketches and a dot product performed even better.

Discussion and Recommendations

The percentage of students that correctly answered questions 3 and 4 was significantly greater than that for questions 1 and 2. Questions 3 and 4 deal more directly with the geometry of slip and a simple calculation, whereas questions 1 and 2 not only require students to understand the differences between elastic and plastic deformation but also to understand how the physical origins of each relate to atomic bonding and dislocations. In addition to understanding the definition of a simple edge dislocation and a 1-D description of its glide motion, students are also indirectly asked about the elastic stress and strain fields around the dislocation core. For example, the nanowire cannot store dislocations because its small volume means that a free surface will always be within close proximity, whereas a macroscopic sample has a significant initial dislocation density that will continually increase as the sample strain hardens during deformation. Since this laboratory is the first time many of the students are exposed to these concepts, their varied responses to question 2 are not surprising.

The questions are then (1) how does the students' use of MD simulations correlate to their responses on the exam questions and (2) what changes can be made to improve student performance. For exam question 1, only 46.8% correctly identified that the elastic modulus should be similar for a bulk copper tensile specimen and a copper nanowire, even though students found, reported, compared and explained the relationship between Young's modulus for each of these specimens in the laboratory activities and reports. By a simple recall of their work performed, all the students should recognize that Young's modulus is similar for both macro- and nano-scale copper specimens. Interestingly, all of the students that correctly answered the first part of the question also correctly answered the second part (Table 2, answer b-iv) suggesting an understanding of elastic deformation as defined in learning objectives 3 and 6 (Table 2) was achieved. We recommend highlighting the Young's modulus relationship again in the post-lab lectures and discussions.

Conversely for exam question 2, most students correctly answered the first part of the paired question but not the second part (Table 3, answer a-v). The concept of dislocation motion (learning objective 4, Table 2) was introduced during the laboratory as the students completed their worksheets (Figures 2 and 3) as a group activity and as part of their group report. The students' performance on the group reports[11] was better than that on the exam. We note that the lab worksheet used conceptual questions that could be answered numerically or with a sketch while the individual reports used questions that asked students to explain their reasoning for the differences in yield stress between the Cu tensile specimen and the Cu nanowire. We recommend including a set of questions in the individual reports that require students to make both numerical calculations and provide schematic pictorial descriptions related to the presence of dislocations and their motion by slip.

For exam questions 3 and 4, student confusion could be addressed without simulation use, but the MD simulations allow students to directly visualize the orientation of the slip plane, as shown in Figure 1. This visualization of slip planes was called upon in both the group activities and the individual reports when students compared their predicted slip plane orientation, based on calculations related to Schmid's law, with the slip plane orientation observed in their nanowire simulations.

Their lower performance on question 4 appears to be related to confusion in how to define the slip plane orientation rather than a lack of understanding of what constitutes an active slip system (learning objective 5, Table 2). We recommend specifically reviewing the angular relationship between Miller indices of planes and directions in cubic systems, using both numerical and graphical solution methods, with emphasis given to the cases of perpendicular and parallel orientations. Performing Schmid's Law calculations in the tensile laboratory is one of the first applications of the knowledge of planes and directions that students learned in the prior crystallography laboratory, and we recommend that these two labs be better linked.

While not rigorously analyzed here, student responses to individual lab report question 5, asking them to generate questions they have about the MD simulation output with regards to understanding plastic deformation at the atomic scale for macro- and nano-sized specimens, indicate that this hybrid lab is causing students to think more deeply about some conceptual questions that would not arise from a lab that does not involve simulation. For example, several students had questions about the accuracy and practical use of simulations and they posed a number of thought-provoking *What if?* questions, that could be answered by virtual experimentation. We recommend that a discussion of these questions be included in the post-lab lecture and certain ideas followed-up with in a subsequent lab that would revisit simulation use.

Conclusion

The collaboration between the MSE and ENE faculty has led to a refinement of the learning objectives for the lab and also to improvements to the nanowire simulation tool. The integrated approach using MD simulations with a traditional tensile testing laboratory completed by second-year Materials Science and Engineering students at Purdue University encourages students to think about the atomic-level processes associated with plastic deformation as they describe and report the macroscopic yield phenomena observed in their tensile tests. This work has helped resolve which concepts students struggle with as they first learn about the atomic-scale mechanisms related to plastic deformation of crystalline solids.

The concept of dislocation motion was introduced with the visualization of the slip process observed in the simulation. Students were able to demonstrate a basic understanding that dislocation motion is responsible for plastic deformation, with slip being driven by shear stresses. Students had reasonable success demonstrating their atomic-level understanding of the forces responsible for the Young's modulus of elasticity, but their selections of the reasons why the nanowire has a greater yield strength than a macroscopic specimen were much more varied.

In this hybrid lab, students are exposed to some higher-level concepts as they are introduced to the basic definitions for crystallography, defects, and plastic deformation. Students should then have a better conceptual foundation when they tackle these concepts again. For example, later in the same laboratory course (*MSE 235*), students study changes in the microstructure and strength of copper and brass specimens as these materials are cold-rolled and subsequently annealed. The concepts of strain hardening and dislocation density could be discussed using relationships introduced in the tensile laboratory, and students could be asked to explain why the nanowire strain-softened instead of strain-hardening.

Recommendations are to highlight the key relationships for Young's modulus and yield strength and to review and discuss students' questions regarding MD Simulations and the atomic nature of plastic deformation during the post-lab discussions; to prompt students to both calculate dot products and draw sketches when working out geometrical relationships for slip systems; and to revisit the results from the MD simulations in the subsequent strengthening mechanism laboratory that occurs later in the same course. These curricular actions would enable students to revisit these concepts to solidify correct understandings and mitigate misconceptions.

Acknowledgement

This work was made possible 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.

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