AC 2010-1263: STUDENT UNDERSTANDING OF ATOMIC BONDS AND THEIR RELATION TO MECHANICAL PROPERTIES OF METALS IN AN INTRODUCTORY MATERIALS SCIENCE ENGINEERING COURSE

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Student Understanding of Atomic Bonds and their Relation to Mechanical Properties of Metals in an Introductory Materials Science Engineering Course

Abstract

We report on initial findings of a project to identify, study, and address student difficulties in a university-level introductory materials science course for engineers. Through interviews of over 80 students and testing of over 300 students, we examined in detail student understanding of the atomic bonding and mechanical properties of metals. Here we describe a number of student difficulties in understanding atomic bonding and its relation to macroscopic properties of metals. For example, students often confuse density, strength of atomic bonds, melting temperature, and yield strength. Many students also believe that when the temperature of a metal bar is increased, the metal expands "because the atoms are moving faster and need more room". Students also often believe that bonds themselves can be permanently weakened or stretched, and they often confuse bond strength with force rather than energy. All of these results were obtained after traditional instruction that explicitly covered these topics. We describe active learning group-work lessons aimed at improving student understanding of atomic bonding which are similar in structure and style to lessons shown to be effective in physics education research efforts. Students were presented with an asymmetric atomic bonding potential energy curve and a symmetric potential energy curve for a "ball and spring" model of atomic bonding. They were then asked a series of questions comparing the behavior of the atoms in the two cases. This lesson was pilot tested in recitation sections, and we found students to be actively engaged in the exercises. At the end of the session students were able to explain on an atomic level why a metal expands when heated, the origin of elasticity of metals and why melting occurs when the temperature reaches a critical level. Previously, most students could not provide these explanations after traditional instruction.

Introduction

Understanding atomic bonding and its relation to macroscopic material properties is a fundamental concept necessary for a basic understanding of materials science. In this paper we describe some of the initial findings of a project to identify, study, and address student difficulties in a university-level introductory materials science course for engineers. In particular, we describe a number of student difficulties in understanding the atomic structure and atomic bonding in metals, and the relation between the atomic bonding and structure and macroscopic properties of metals. In addition we briefly describe some pilot instructional materials developed to help overcome these student difficulties.

There are a several previous studies, including the development of a Materials Concept Inventory, that have identified and described some student difficulties with understanding atomic bonds and/or their relationship with material properties¹⁻³. In an initial phase of this study, we administered the Materials Concept Inventory, which covers a wide range of topics, and found similar levels of student difficulties with atomic bonding. This current study was aimed at investigating these and related difficulties in more detail. Here we report on our findings of additional student difficulties with atomic bonds and materials properties and characterize in more detail the student difficulties with this topic found in some of these earlier studies.

Participants and methods

The participants in this study were enrolled in the introductory materials science course for engineers at a public research university, a required core course for many of the engineering major programs. The students ranged from 2^{nd} to 5^{th} -year students and about 10% of the students intended on becoming materials science engineering majors.

Data was collected over a period of 4 quarters, with approximately 160 students per quarter, and was collected in three ways. First, midterm and final exam data was collected. The exams were in multiple choice format and some of the items (about 10-20%) were designed by us in collaboration with the instructor. These items were aimed at testing specific student difficulties with the course material. Second, for two of the four quarters, volunteer students were recruited for testing and interviews. These students received a small amount of extra credit and the opportunity to volunteer was offered to all students in the class. Approximately 25% of students volunteered in these quarters. The volunteers participated in a one-hour session in which they were interviewed for part of the session and tested in the remaining portion. The test items consisted of multiple-choice or free response-format.

The third method of collecting data integrated student participation more directly into the course. In addition to the standard homework, students were also given a "flexible homework" assignment with credit for participation as part of the course grade. The flexible homework assignment consisted of participation in a one-hour session in our research lab where students would complete some combination of testing and interviewing. Several times during the quarter, we would randomly select a recitation section, and ask students to sign up for flexible homework. Typically, about 95% of students participated in the flexible homework. Those students who did not wish to come to an interview/test session were given the opportunity to complete a one-hour homework assignment. During the flexible homework session, students were told to answer the questions as best they could, even if they have not yet seen the material. For the testing portion of the session students sat at individual stations in a quiet room. The tests items were in either multiple-choice, free-response, or a multiple-choice-with-explanation format. Students completed the material at their own pace. Afterwards we would informally ask students whether they had any questions and/or to explain their answers. We observed during these sessions that students made a good faith effort to answer the questions to the best of their ability. For the interview portion of the sessions, students were in a separate room. Some of the interviews were video and audio recorded. About 60% of the students were interviewed individually, the rest were interviewed in groups of 2 or 3. Most of the test data and interviews were at least one week after the relevant instruction, however, some were given before the relevant instruction in order to determine pre-instructional knowledge. The data reported here is all post instruction.

Student beliefs about density, atomic separation and atomic bonding

Students often believe that the density of a material determines some of its physical properties. For example, Figure 1 shows that 64% of students answered that a more dense material will have a higher melting temperature. Another example is shown in Figure 2, in which 20% of students answer that a metal rod drawn through a tapered hole increases in strength because its density increases (this question is somewhat similar to an item on the Materials Concept Inventory). It is interesting to note that the question in Figure 2 was administered several weeks after an identical question was given on the midterm (with similar answer patterns) and students were given the opportunity to correct their answers.

Material A is denser than Material B. How does Material A's melting temperature compare to material B's.

- a) Material A has a higher melting temperature than Material B.
- b) Material A has a lower melting temperature than Material B.
- c) Material A has an equal melting temperature than Material B.
- d) Not enough information.



Figure 1. Student response percentages to the indicated question. N= 52. Error bars represent standard error of the mean.

Two thin metal rods are cut from the same plate. Rod A is pulled through a tapered hole smaller than the rods original diameter. Nothing is done to Rod. B.

- a) Rod A has a higher yield strength than Rod B because it has more defects.
- b) Rod A has a higher yield strength than Rod B because it has become denser.
- c) Rod A has a lower yield strength than Rod B because it is now thinner.
- d) Rod A has a lower yield strength than Rod B because it has already been under stress.



Figure 2. Student response percentages to the indicated question. N= 51. Error bars represent standard error of the mean.

Why do students believe that higher density implies higher melting temperatures and higher strength? We found four different yet somewhat related reasons. First, many students apparently believe that the bond strength depends on atomic separation. In particular, many students believe that as atomic separation decreases, the bond strength of a material increases. For example, 23 students were asked to write an explanation for their answer to the question comparing melting temperatures of two materials with different density, given in Figure 1. For the students choosing the denser material as having the higher melting temperature, a very common explanation (>80%) was similar to the following responses:

S1: "Since A is denser, the atoms are closer together, therefore it takes more energy to break the bonds."

S2: "Closer packed (denser) material will have stronger atomic bonds b/c they are closer together thus allowing the interacting forces to be stronger."

Evidence of the student belief that density is related to bond strength is further supported by student responses to another test item given to a different (randomly chosen) group of students. The item was in free-response format and posed the following question: "Does a material which is denser have stronger atomic bonds than a material which is less dense?" A typical student response was:

S3: "A material that is denser is stronger because they have shorter ave. bond length then less dense materials"

S4: "A material which is denser has stronger bonds because the atoms are tightly packed."

Notice that S3 didn't answer the question about stronger atomic bonds, but rather said the material is stronger, presumably because the student is either equating bond strength with material strength, or he/she is not aware that a distinction needs to be made between them. A number of students made this same mistake. Furthermore, the response of S4 and S2 brings up another potential issue. Students seem to be confounding the ideas of density, close-packed, bond strength, and material strength all together. For examples, while students are told in lecture that close-packed structure tends to result in a stronger material, student responses appear to imply that many interpret the reason for the increased strength incorrectly. Many students will (incorrectly) reason that close-packed materials are stronger than non-close-packed because close-packed bonds are necessarily stronger, which is not only incorrect, but also disregards the idea that material strength depends on the slipping of atomic planes.

The second reason for linking density and melting temperature is based on a pervasive erroneous assumption that as the density of a material increases, atomic separation decreases. Examples of this are in all of the quotes above. In fact, the overwhelming majority of students made this assumption. These students could have interpreted (implicitly or explicitly) that "density" means "number density" rather than the more commonly assumed "mass density". The focus on number density might be expected, since the lessons on crystal structure focus on numbers of atoms, for example when calculating the atomic packing factor, rather that the mass of the atoms. While this may not be a large problem itself, as students usually recognize the difference between mass

density and number density when prompted, the fact that the students do not think carefully about using density without being prompted may lead to errors in solving larger problems.

The third reason is less obvious, but it appears that some students reason that since the atoms are more closely packed in a dense material (incorrect), then the melting temperature must be higher because atoms need to be far apart to be a liquid. Thus they incorrectly conclude that the atoms must separate more for a higher density material, which requires higher temperature. This is somewhat apparent in the following student's written responses to two free-response questions. The first is a free response version of the question in Figure 1.

S5: "Tm of mat A is higher because atoms must move farther away before melting occurs."

While this response has some elements of correct thinking, the response by the same student to the subsequent free response question "What is meant by 'stronger atomic bonds'?" reveals that this student is probably not thinking (incorrectly) that the closer atoms have stronger bonds, rather that closer atoms need to be separated more in order to melt.

S5: "Stronger bonds require more energy to break, I don't think atomic bond length affects bond strength" I don't know how density affects the strength of atomic bonds."

This student has some correct understanding, but is clearly still confused about the relation between density, bond strength, atomic separation and the conditions required for melting.

Finally, there is a more subtle fourth reason why some of the students may think that a higher density material has a higher melting temperature. There is evidence that some of the students are confusing temperature with thermal energy. For example, explaining the response choice D (correct) to the multiple question in Figure 1, a student wrote:

S6: "For a dense material there are more bonds, more bonds require more energy to the system and more energy required means the temperature will need to be higher. But different materials have different material qualities So D because it does not say they are the same materials."

Clearly, this student is thinking that temperature scales with the total energy of the system rather than the average energy per particle. Therefore the reasoning is that more energy is needed to heat up the dense material (correct), thus more heat means higher temperature (not necessarily correct). The student obtained the correct answer, but there is clearly a misconception in part of his/her reasoning. There is evidence that a significant number of students were thinking this way, though their answers were more ambiguous. For example a typical response was:

S7: (chose: A, incorrect) "Melting temps will certainly be different. Since Mat. A is denser, it will require more energy to melt."

From the written responses and interviews, it was clear that many of these students probably did not have a clear picture of their own reasoning. Nonetheless, a significant number of the students were confusing heat and temperature, a fairly common student difficulty (e.g., see Ref. 4), and it is interesting to note that this issue is manifest here.

Student beliefs about the nature of atomic bonds in metals

Weakened bonds

We have observed a number of interrelated incorrect beliefs or "misconceptions" that students have about the nature of atomic bonds. Many of them seem to stem from macroscopic analogies. For example, during student interviews, we asked some students the question: "Why does a metal get softer when heated?" A typical response was "because the bonds get weaker when heated". When asked to clarify, students typically explained that the bonds themselves were getting weaker (somewhat like springs between the atoms getting softer, more pliant), and this is why the metal is softer. There was no mention of bonds breaking or movement of dislocations. Rather, the students often believed that the strength of the material is derived directly from the strength of the bonds, and heating up the bonds makes the bonds weaker. This result is consistent with findings in a similar study².

Further support of this idea of weakening bonds comes from student responses to why a metal expands when heated, in Figure 3. Over 36% of the students choose response D, explaining that the metal expands because the bonds weaken, allowing the atoms to move farther apart. Many students also choose B, explaining that the atoms move faster and with greater amplitude, and they need more room to do this, which is perhaps a better choice than D, but still unsatisfactory.

When a metal is heated, it expands because the average atomic separation between adjacent atoms increases. Which of the following is the most accurate explanation for why this happens?

- a) The increased temperature lowers the melting temperature, resulting in increased separation of the atoms.
- b) The atoms move faster and with a greater amplitude, and more space is needed to allow for the increased movement.
- c) The asymmetry in the atomic bonding potential causes atoms to move farther apart when their energy increases.
- d) As the temperature increases, the atomic bonds weaken, allowing the atoms to move farther apart.
- e) As the temperature increases, the atoms expand in size, thus the metal expands.



Figure 3 Student response percentages to the indicated question. N= 52. Error bars represent standard error of the mean.

Stretched bonds

A significant number of students also believe that atomic bonds can be permanently stretched. During interviews we asking some student the question: "Draw an example of atoms in a metal before and after the metal has undergone plastic deformation". A small but significant number of students ($\sim 10-20\%$) drew atoms permanently farther apart in the post-deformation sketch and explained that the bonds between the atoms were stretched (much like a spring can be permanently stretched).

Further support of the stretched-bond misconception is shown in Figure 4. Students were asked to compare the volume of a metal before and after plastic deformation, and 30% of them choose A, that the volume of the metal would be greater after deformation. Note that this idea of stretched bonds may be similar to the results found by Krauss et al.² for a question in the Materials Concept inventory, in which many students answered that when a wire is drawn through a tapered hole, the bonds have been compressed.

A metal bar experiences tension stress and deforms plastically: when it is released from tension, it is longer than its original length. If the volume of the bar is initially V, what is the volume of the bar after it is stretched?

- a) greater than V
- b) equal to V
- c) less than V



Figure 4. Student response percentages to the indicated question. N = 68. Error bars represent standard error of the mean.

Describing Bond Strength: Energy or force?

Atomic bonds are often described by instructors as being either "strong" or "weak". Unfortunately this can be misleading or confusing to the student because sometimes the word "strong" refers to the force of the bond and sometimes it refers to the bond energy. Like many misconceptions, the use of a common word can lead to difficulties in understanding the proper scientific concept. In everyday usage, "strength" usually refers to force, whereas normally when an expert speaks of a strong atomic bond, it is meant in terms of a large binding energy. This confusion is reflected in student responses. For example, in a free response version of the question in Figure 1, comparing melting temperatures of materials with different densities, a student wrote: S8: "[The higher density material has higher melting temperature] because there are more atoms packed closer together which will require more energy to separate them."

However the same student in a answering the following question "What is meant by 'stronger atomic bonds'?" (which was two questions after the above question) the student writes:

S8: "Stronger atomic bonds is the attraction force between the atoms."

Thus in one context regarding the extent to which the atoms remain bound, the student refers to energy, and in the other the student refers to force. In another example, a different student reverses the context in which force and energy are used. When comparing melting temperatures and density the student writes

S9: "[*The higher density material has higher melting temperature*] because the bond lengths would be shorter, meaning the atoms are pulling on one another much more."

However, when answering the question "What is meant by 'stronger atomic bonds'?" the student refers to energy instead of force:

S9: "The E_0 is very low meaning it would take a lot of energy to break the bonds. A denser material would have stronger bonds."

In general we observed in interviews that it was common for students to switch between arguments using force and arguments using energy, with little regard for the scientific accuracy of their own usage of the words or concepts.

Addressing student difficulties: a sample exercise

The previous sections described a complicated, interrelated array of student difficulties with understanding about atomic bonding and its relation to material properties. The main purpose of this paper is to describe students difficulties, however, here we briefly describe a preliminary pilot sample exercise to help students address a small subset of these difficulties. The exercise is intended to be completed by students in small groups of 3 or 4 in a "recitation" type format. The recitation instructor(s) do not lecture, rather leave the students to complete the task and pose questions to individual groups when they have problems.

The exercise focuses on student understanding of the potential energy of two metal atoms as a function of separation. We chose this topic for several reasons. First, a basic (and we stress *basic*) conceptual understanding of the major features of the potential is fundamental to understanding the nature of atomic bonds and this can be used throughout the course. In fact the curve is presented and explained in a standard introductory materials science textbook⁵. Second, the graph is a convenient visual representation that facilitates understanding of the separability of the fundamental dimensions of bond energy, average separation, and curvature that can be conceptually linked to macroscopic properties such as melting temperature, density, and elasticity. This can help students to more clearly distinguish between ideas such as atomic

separation and bond energy as well as yield strength (related in part to depth of well) and elasticity (related to curvature of well).



Figure 5. Diagrams of the "atomic bond model" (i.e. Lennard-Jones potential) and the "spring model", given in a recitation group exercise. Students compared the atomic behavior and subsequent material properties of the two models. For example, students are asked, "What happens to the average separation for the spring model and atomic bond model when E_N increases?"

The exercise consists of a brief explanation of the two models presented in Figure 5. Students are asked a number of questions that compare the properties of the two models. This includes describing and comparing the motion of the atoms in the two cases, and how the average separation between the atoms changes when the average energy increases. Student are also asked to discuss in detail how the Lennard-Jones potential is related to melting temperature, Young's modulus, coefficient of thermal expansion, and the energy necessary to break bonds as a function of temperature. We found that even though these concepts were mentioned in the textbook and in Lecture, most students were not at all familiar with the potential or how it is related to the behavior of the atoms and the mechanical properties of materials.

We have piloted this exercise in five recitation sections in one lecture class. From observations of the recitation classes, we found that the students were engaged with the exercise, and most were able to relate the potential and atomic bonding to macroscopic properties as well as properly explain why a metal expands when heated by the end of the recitation class. To this extent the pilot was a success. However, results on a midterm several weeks after instruction revealed that only about 25% of the students correctly answered a relevant question about the material. Therefore, we are in the process of modifying the exercise to improve performance.

Summary and Discussion

We have identified a number of student difficulties with understanding basic concepts regarding the nature of atomic bonds in metals and how the characteristics of the bond help to determine macroscopic properties such as elasticity, melting temperature, thermal expansion, and density. Many of these difficulties and "misconceptions" remain after traditional instruction. From a broad perspective, we found four main student difficulties. First, a persistent and common web of incorrect beliefs held by students both before and after instruction is that denser materials have atoms with smaller separations, and this smaller separation results in stronger bonds between the atoms, in turn resulting in higher melting temperature and stronger materials. Second, students typically confuse the ideas of force and energy when reasoning about the "strength" of atomic bonds as well as how this translates to macroscopic properties. Third, many students believe that the atomic bonds themselves are permanently changeable. Analogous to a bond acting like a physical spring, many students believe that the bond may permanently stretch or weaken. Finally, we found that few if any students were able to explain on an atomic level the cause of thermal expansion in metals.

While the main purpose of this paper is to describe some student difficulties in learning materials science, we also briefly discussed a preliminary effort to address some of these identified difficulties. Our strategy to address these difficulties included detailed exercises involving comparisons of the asymmetric Lennard-Jones potential and the symmetric spring potential. We found that students did not have even a simple understanding of this representation of the atomic bond, even though it was presented in lecture and in the textbook. While there is clearly room for improvement, the exercises were an excellent vehicle for eliciting the previously mentioned misconceptions and facilitating better understanding of atomic bonds and their relation to macroscopic properties.

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Bibliography

1. Krause, S., Decker, J.L., and Griffin, R., "Using a Materials Concept Inventory to asses conceptual gain in introductory materials science courses", *33rd ASEE/IEEE Frontiers in Education Conference Proceedings*, 2003.

2. Krause, S., Tasooji, A., and Griffin, R., "Origins of Misconceptions in a Materials Concept Inventory From Student Focus Groups", 2004 ASEE Annual Conference and Exposition Proceedings, 2004.

3. Kitto, K. L., "Developing and Assessing Conceptual Understanding in Materials Engineering Using Written Research Papers and Oral Poster Presentations", *38rd ASEE/IEEE Frontiers in Education Conference Proceedings*, 2008.

4. Strevler, R. A., Litzinger, T. A., Miller, R. L., & Steif, P. S., "Learning Conceptual Knowledge in the Engineering Sciences: Overview and Future Research Directions" *Journal of Engineering Education*, 2008.

5. Callister, W. D., Materials Science and Engineering: an Introduction, Wiley, New York, 2007.