Introductory Material Science: A Solid Modeling Approach

Gerald Sullivan
Department of Mechanical Engineering, Virginia Military Institute

Abstract

As a means to enhance students' abilities to visualize the three dimensional structure of materials, solid model based exercises have been integrated into the introductory materials science curriculum at the Virginia Military Institute. The exercises included exploration oriented tasks, where students used the viewing functions of the solid modeling environment to examine models of materials, as well as problems where students constructed their own models of materials. The intent of the exercises was to allow students to obtain a deeper understanding of the three dimensional structure of materials, while at the same time reinforcing their solid modeling skills. This paper reviews the exercises developed to complement the materials curriculum, and describes the lessons learned in this first attempt at applying solid modeling as a visualization tool for material science education.

1. Introduction

Material science is an extremely diverse body of knowledge, comprised of concepts ranging from quantum level interactions between atoms, to explanations of the effects of industrial processes on material properties. Central to the understanding of these concepts is the ability to visualize and reason about the somewhat abstract three-dimensional arrangements of atoms that make up the structure of materials, (e.g. crystal solids, amorphous solids and polymer chains). In many cases students taking their first material science course do not have adequate 3-D visualization skills [1], and are unable to develop a deep understanding of the principles responsible for the behavior of engineering materials. As a means to supplant weak visualization skills and improve comprehension of material science concepts, the mechanical engineering department at the Virginia Military Institute has incorporated solid modeling exercises into the material science curriculum. The intent of these solid modeling exercises is to help students interactively explore the crystal structures that make up metallic substances, in an environment that amplifies the students' abilities to operate in an abstract 3 dimensional landscape. In addition to supporting the material science curriculum, the inclusion of solid modeling exercises in the materials science class also supports the equally important goal of improving students' long-term retention of solid modeling skills. In the paper that follows, a description of the current material science program at VMI is given, along with a summary of characteristic problem areas for student comprehension in material science. Goals for the incorporation of solid modeling tools with the materials science course are reviewed, and descriptions of solid modeling exercises are detailed. Lastly, student reactions to the new teaching approach are discussed, as well as future plans for using solid modeling in the materials course.

2. Background and Goals

Currently the mechanical engineering dept. at the Virginia Military Institute offers an introductory material science course for their second year students, during the fall semester. The course begins with an over view of material properties and introduces elastic and plastic deformation, as well as brittle fracture. This first section of the course emphasizes the characterization of material behavior via material properties, and is backed up with extensive laboratory experimentation, (e.g. tensile tests, torsion tests, charpy impact tests). The next section of the course goes beyond characterizations of material behavior and investigates the mechanisms responsible for the observed behavior of materials. During this part of the course the links between macroscopic properties of materials and features of the materials microstructure, crystalline structure and atomic structure, are presented. The goal is to provide students with the ability not only to describe material behavior but also to predict behavior based on information about the structure of the material on microscopic and atomic scales. Finally in the last section of the course, students are given a basis for manipulating material properties through an understanding of equilibrium and non-equilibrium phase transformations, as well as an introduction to industrial heat-treating practices.

By far the most difficult concepts for students to grasp in this course are those involving the relation of macroscopic material properties to the microscopic and atomic scale features of a material. In large part, the problems can be traced to students' difficulty in visualizing the three dimensional structure of materials at the atomic level. Key material science concepts that are directly related to the 3-D crystalline structure of metals include anisotropy/isotropy, elasticity, and plasticity. The inability to visualize and manipulate the 3-D crystalline geometries associated with structure of metals, prevents students from gaining a true appreciation and understanding of these concepts.

Recognizing this issue, authors and publishers of textbooks, now include software with their textbooks to help students probe the structure of unit cells for a variety of materials, [2]. Students gain some improvement in their understanding of the structure of materials, but the limited scope of the software bundled with texts, does not provide all of the features and tools that allow truly interactive study of material structures. Particularly useful features that are not available in the software that accompanies textbooks include:

- modeling primitives that allow students to generate new geometries
- advanced viewing features that allow students to generate sectional views of structures at any point and orientation in space within a crystal structure
- A full complement of measurement tools that permit students to find distance, area, and volume measurements within a crystal structure

As an alternative to these relatively simplistic software aids, some universities are now using sophisticated 3-D visualization environments to allow students to probe the inner structure of materials [3],[4]. At Valparaiso University, the Visbox virtual reality environment is used as part of the materials curriculum to view crystal structures of metals and ceramics, as well as the structure of polymer chains, [5]. The resolution of this tool is so powerful that it may even be used by students to examine the details of the orbital structures within the atoms of a material. This option does provide almost limitless potential for interactive study of material structures, however, has the disadvantage that dedicated equipment must be purchased, and lab space provided in order to implement the technology. To justify this approach, multiple courses would have to incorporate the visualization environment in their curricula requiring extensive coordination and expenditure of time by faculty.

In the materials science course at the Virginia Military Institute, an attempt has been made to provide interactive visualization tools for the materials course by leveraging our existing investment in solid modeling software, (Autodesk Inventor), and workstations. Students at VMI, as well as in many other engineering programs nationwide are first exposed to solid modeling technology during their first year in the engineering curriculum. At VMI, the introductory materials science course follows the solid modeling course during the first semester of students' second year in the mechanical engineering program. It was felt that since the materials science course followed immediately after the solid modeling course, students would still retain enough knowledge of solid modeling to use it effectively in the materials course. Pedagogically, this sequence has the advantage that material science concepts are strengthened, while at the same time solid modeling skills are rehearsed and refreshed, aiding in their long term retention. This type of longitudinal incorporation of concepts across the curriculum has been gaining popularity at universities in the US, and is the basis for the "Spiral" engineering curricula now being pioneered at University of New Haven, [6]. Educators at the University of New Haven have found that by moving to course sequence that constantly revisits multiple sets of skills and concepts, students do demonstrate better retention and additionally are better able to operate in multidisciplinary teams. Incorporating solid modeling into the materials course at VMI represents just a single case of networking two courses together, however, with a small incremental effort, the approach could be adopted for other visualization intense courses, (statics, design, strength of materials).

In the materials science course at VMI, the primary expectations for the use of solid model based exercises were as follows:

1. Allow students to use solid models of crystal structures in an explorative mode, panning, rotating and zooming in on important features of the crystal structures.

2. Allow students to generate views of crystal structures on arbitrary planes and point in space.

3. Use distance, area, and volume measurement tools available in the solid modeling environment to analyze the geometry of crystal structures and planes.

4. Allow students to model crystal structures on their own, using the geometrical construction features and mating primitives available in the solid modeling environment.

It was felt that these expectations were well aligned with the skill set covered in the solid modeling class, and at a reasonable level of difficulty for students. With only four months between the completion of the solid modeling class and the beginning of the materials course, it was anticipated that students would be able to jump back into solid modeling with a minimum of retraining necessary. In the end analysis, this assumption was not completely accurate and forced a rethinking of how solid modeling should be used in the materials curriculum.

3. Summary of Exercises

The solid modeling exercises for the introduction to materials class at VMI were first introduced into the curriculum during the fall of 2004. The exercises planned for the course along with their objectives are listed as follows:

1. **Cubic Crystal Structures**: As a companion to the lecture material pre-built models were provided to the students to allow them examine the unit cells and lattices for Simple Cubic, Body Centered Cubic and Face Centered Cubic crystals. Facility with panning, rotating and zooming functions were the only skills required to allow the students to fully explore the spatial relationships between the atoms in these structures. The exercise helped students in understanding:
    - What a unit cell is
    - Where are atoms actually located for a given crystal structure
    - What atoms actually touch in the unit cell, and what is the direction along which the atoms touch.

2. **Hexagonal Close Pack Structure:** In this exercise students build a solid model of the unit cell for a hexagonal close pack structure, and then use the measurement tools available in the solid modeling environment to calculate the atomic packing factor. The packing factor was then compared to the packing factor for the FCC structure presented in lecture. Students were also required to generate section views on various planes of the HCP structure to look at the difference between closest packed planes in the structure and planes that are not closest packed. This particular geometry is usually difficult for students to analyze mathematically because they do not have a fundamental understanding of how the atoms of the HCP structure nest together in three-dimensional space. “Building” the structure a layer at a time makes the relationships between the atoms that make up the HCP structure clear. Additionally, because students generate a model of the structure, they do not have to rely on sometimes lacking mathematical skills to determine the distances between key features in the HCP structure. In this exercise, required solid modeling skills included building up assemblies using mating primitives, as well as using measurement tools and creating work planes and section views. Specific material science concepts that this exercise demonstrated were:

- How atoms in a hexagonal close pack unit cell coordinate with one another.
- Atomic packing factors for closest packed crystal structures
- How atoms are arrayed in different planes of the HCP structure

3. **Crystallographic Planes:** FCC, BCC crystal models were given along with predefined work planes that correspond to different crystal planes. Students were to activate different section views to reveal the structure of atoms in each plane. Students were then asked to generate views on planes defined by a given set of miller indices. In this exercise, it was expected that students be able to create section views and define work planes in the given models of crystal structures. Concepts illustrated by the exercise included:
    - Understanding miller indices
    - Appreciating the difference in the planar geometries for different crystal structures

4. **Families of Planes:** Models of FCC and BCC crystal structures were provided with pre-defined work planes corresponding to the {101} and {111} families of planes. Students were to generate section views on each of the planes corresponding to a given family and crystal structure. On each plane measurements of the distances between atoms were taken. Concepts demonstrated in this exercise included:

    - The idea of equivalence between geometrically different planes in a given crystal structure
    - The concept that the family of planes is dependent on the crystal structure. For example, the {111} family in the FCC structure contains different planes than the {111} family in the BCC crystal structure.

5. **Relationships Between FCC and HCP Structures:** In this exercise, students looked at successive {111} planes in a model of an FCC lattice that was provided for them, and compared it to the {0001} planes of a model of an HCP lattice. Specific goals for this exercise were:

    - For students to see and understand the packing sequence of closest packed planes in an FCC structure. This is typically a confusing concept for students, but with appropriate section views through an FCC lattice, the three layer stacking sequence, (ABCABCABC…), becomes clear.
    - For students to understand the stacking sequence in the closest packed HCP structure, and to recognize the relationship between FCC structures and HCP structures. This is especially useful at a later point in the course where stacking fault defects are described.

6. **Dislocation Structures:** In coordination with students' first exposure to the role of dislocations in plastic deformation, an explorative exercise was given in which students examined models of edge dislocations and screw dislocations. Two

dimensional chalk board depictions of dislocations presented in lecture, and the isometric views of dislocations found in texts, do not fully illustrate the geometry of these important defect structures. In particular students have difficulty in understanding why a dislocation is a "line defect", and where in the crystal structure the line defect actually resides. In this exercise, solid models of edge dislocations and screw dislocations are provided to the students. They are asked to use the pan, zoom and rotation functions as well as section views to determine where the dislocation line is for both the screw and edge dislocations. In comparison to the other exercises, the required level of expertise in solid modeling is minimal; the primary goal is to develop a qualitative understanding of dislocation geometry.

7. **Slip Planes and Directions:** The purpose of this exercise was to emphasize the relation of crystal structure to plastic deformation and ductility by having students look at the slip systems in FCC and HCP crystal structures. Using the work plane construct and measurement tools available in the Autodesk Inventor package, students were asked to find the distances between atoms on given slip planes and slip directions. They were then asked to find the distances on other planes and directions within the three-dimensional crystal structure on which slip does not occur. Based on the observations from the model, students were asked to comment on the features that characterize slip planes and directions. The primary concepts illustrated by this exercise were that:

    - Slip typically takes place on the most densely packed crystal planes in the directions where atoms are the closest together. Using solid models to study the places that slip does and does not occur establishes the concept of a slip system.
    - Different crystals structure, (HCP and FCC), have differing numbers of independent slip systems on which slip may take place. This is an extremely important concept since it provides and understanding of the link between ductility and crystallographic structure of a given material.

8. **Solid Solutions:** In the last section of the materials course, solid solutions are presented, with an eye towards using thermal processing to manipulate the mechanical properties of materials. It is at this point in the course where phase diagrams are presented to represent the interaction between the phases of a solid solution as a function of temperature and composition. As a means to explain the shape of single phase regions on a phase diagram, this last exercise examines the solubility of carbon in the phases of iron that occur in steel at different temperatures. Students are given the models for FCC iron, which is the phase of iron that exists in steel at high temperatures, and BCC iron, the room temperature phase for iron. They are then asked to use their solid modeling skills to determine the size of interstitial atoms that would fit into the octahedral sites and tetrahedral sites in FCC and BCC iron respectively. This is a common textbook problem, but using the modeling environment provides more insight into the arrangement of atoms around the available interstitial sites. In addition the use of solid modeling tools makes it easier

for students to determine the size of the interstitial atom that could fit into one of the sites without straining the lattice. Solubility of carbon in the different phases, and thus the shape of the associated single-phase regions on the phase diagram can then be motivated as a function of larger amount of space for interstitial solute atoms available in the FCC iron as compared to the BCC iron.

At the time these solid modeling exercises were conceived, there was no available measure of the proficiency of students with the Autodesk Inventor solid modeling package. Based on their relatively recent exposure to solid modeling, it was assumed that students would be able to carry out any of the exercises described above without additional coverage of solid modeling concepts in class. As the course evolved it became clear that the majority of the students' skills with Inventor were not adequate to handle many of the proposed exercises. As a result, some of these exercises were modified, adopted as demonstrations, or dropped all together. In the section that follows, more detailed information as to the reaction of students to the solid modeling exercises is given, along with plans for future use of solid modeling tools in the materials course

4. Student Reactions and Plans for the Future

The primary goal of the exercises described in the previous section was to provide a 3-D visualization environment for helping students to understand materials science concepts. As there was no intention to cover solid modeling concepts in the materials science lecture time, it was essential to the success of this endeavor that students entering the material science course in the fall semester of 2004 had achieved and retained a reasonable degree of fluency with the Inventor solid modeling package. In practice, it was discovered early on in the materials course that the class could be divided into two groups based on their level of achievement with solid modeling:

1. Students who had not mastered solid modeling skills, or were not able to retain their solid modeling skills

2. Students with a good working knowledge of solid modeling.

Population wise, about 80% of the class fell into the first category, (i.e. those students that did not have usable solid modeling skills), with only 20% making up the part of the class with intact solid modeling skills. In general, students in the first category were receptive to more passive uses of solid modeling, (panning, zooming and viewing exercises), while students in the second category were able to perform exercises involving 3-D geometrical construction. As the course progressed it was clear that there were benefits in using solid modeling tools for each group of students, but that the difficulty of the materials science concepts mastered were directly related to the students' solid modeling capabilities. Unfortunately, the majority of the class was unable to take part in the "active" style of solid modeling exercises, (i.e. exercises involving 3-D geometrical construction), which at the outset of the course were expected to have the largest impact on students' abilities to visualize and understand material structures.

The first point during the course where it became apparent that the solid modeling skills of students were not at the level assumed during the design of the exercises occurred when the students were asked to model the hexagonal close pack crystal structure described in exercise 2. It was observed at this time, that the majority of class was unable to use the basic solid modeling constructs that are necessary to generate models of material structures. During office hours and help sessions with students from the class the following difficulties were noted:

- Students could not recall or never knew how to generate construction geometries such as the Work Points, Work Axes and Work Planes available in the Inventor package.
- Students had trouble creating assemblies. In particular, students were confused about defining mates between the "atoms" used to construct crystal geometries.
- Students had difficulties in fully constraining assemblies and often created models that "floated apart" or "imploded".
- Students had trouble in applying measurement tools.

For these students, referred to as "first category" students above, the difficulty and frustration of trying to use the solid modeling environment obfuscated any learning of materials science concepts intended for this exercise.

In contrast to the students in the first category, about 20% of the students in the class made up a second category of solid modeling literate students who were able to carry out the exercise relatively easily. During conversations with these students following the assignment, a frequent comment was that "something clicked" during the modeling process for the Hexagonal Close Pack structure, and that the students could now "really understand how the HCP structure went together". These students also appreciated the ability to take arbitrary section views of their models, and tended to use the solid modeling environment as a means to probe and dissect the HCP structure. Students in this second category had all achieved a "critical mass" with respect to their solid modeling skills and were able to take part in a more operant style of learning than was possible for the other students.

Although students in the first category did not have the skills needed to construct their own models of material structures, they were able to exploit the solid modeling environment in a more passive way, using the panning, rotation and zooming features to view solid models that were provided for them. The first exercise, Cubic Unit Cells, involved the use of viewing operations only, and was straight forward for all of the students in the class. The concepts in this exercise were not exceptionally difficult and in general, the use of viewing operations seemed to provide adequate information for the students. Following the problems with exercise 2, (Hexagonal Close Pack structures), Exercises 3 through 7 were converted to viewing style exercises and demos, while exercise 8 was dropped. In cases such as the exercises 3 and 6, viewing pre-built solid models was of interest to students, and did help with understanding the intended concepts. This was particularly true for exercise 6 where students examined models of edge dislocations and screw dislocations. In this case, the ability to zoom in, and rotate models of dislocations greatly improved students understanding over what would have been possible from static illustrations available in texts. In other cases such as exercise 5, where the goal was to look at the relationships between HCP and FCC structures, merely having students examine "canned" section views within the two crystal structures did not enhance their acquisition of concepts. To understand the concept of stacking sequences in these closest packed structures, students need to understand the orientation of closest packed planes themselves, as well as which direction they must look in to see the pattern of the stacking sequence revealed. Here, as with the modeling of the HCP structure in exercise 2, a more active style of learning is needed, in which the student interacts with the geometry of the model to develop spatial concepts. In comparison with exercises such as the exploration of dislocation structures, this exercise is much more demanding cognitively, and requires a higher level of solid modeling skills on the part of students.

In summary, the use of solid modeling to enhance the understanding of materials science concepts can take place in a fairly low level "viewing mode", or in a more active, operant mode where students actually generate and interact with the solid models of a material structure. While the viewing mode is effective for understanding some spatial concepts, there are many concepts even in the introductory materials science course that require the "active" solid modeling mode. Realizing the full potential that solid modeling tools afford materials science education depends on students coming into the material science course with intact solid modeling skills. To increase the likelihood that this happens in the future the following actions are being taken now in preparation for the students enrolling in the fall 2005 materials course:

- Feedback from the materials course solid modeling experience is being provided to the solid modeling instructors as to the skill set and problem areas of students that have gone through the course.
- Example problems from the material science domain will be injected into the solid modeling course. This will give students some foreknowledge of what they will see in materials and let them iron out some of the problems peculiar to the material models while they are still immersed in solid modeling.
- Development of a primer to guide students through the use of the subset of modeling primitives required for the material science exercises.

5. Conclusions

Solid modeling is one of many possible means by which students may access high-powered visualization tools for studying the complexities of the 3 dimensional material structures. The solid modeling approach has the advantage that is cheap, (most schools already own solid modeling software), and has a rich functionality for viewing and generating models of the atomic structures occurring in materials. Potentially, the solid modeling environment is the ideal medium for demonstrating a variety of material science concepts from basic crystallography to solid solubility. Experience with using solid modeling in the materials course at VMI has shown that poor retention of solid modeling skills greatly limits the scope of the concepts that can be addressed by students. Future attempts at using solid modeling effectively in the material science curriculum hinge on efforts to improve the retention of solid modeling skills by increasing the opportunities for feed back and feed forward of information between the two courses.

7. Bibliography

1. Strong, S. and Smith, R., Spatial Visualization: Fundamentals and Trends in Engineering Graphics, *Journal of Industrial Technology*, November 2001 to January 2002, 18(1), 1-6
2. Callister, W.D., *Material Science and Engineering, an Introduction*, 2002 John Wiley and Sons
3. Dede, C., Salzman, M. and Loftin B., Science Space: Virtual Realities for Learning Complex and Abstract Scientific Concepts, Proceedings of VRAIS ’96, San Jose, CA, pp. 246-252.
4. Kriz, R. D., Farkas, D., and Batra R. C., Integrating Simulation Research into Curriculum Modules on Mechanical Behavior of Materials: From the Atomistic to the Continuum, *J. of Materials Education,* **21**, 47-56, 1999.
5. Will, J.D., and Johnson E.W., Scientific Visualization for Undergraduate Education, *Proceedings of the 2004 American Society for Engineering Education Annual Conference and Exposition*, Session 3138
6. Collura, M.A., Aliane, B., Daniels S., and Nocito-Gobel Jean, Development of a Multidisciplinary Engineering Foundation Spiral, *Proceedings of the 2004 American Society for Engineering Education Annual Conference and Exposition,* Session 2630

Biographical Information

Gerald Sullivan:

Dr. Sullivan, Assistant Professor of Mechanical Engineering at the Virginia Military Institute, received his B.S.M.E. from the University of Vermont in 1985, and his M.S.M.E. and Ph.D. from Rensselaer Polytechnic Institute in 1987 and 1991 respectively. He has held teaching positions at the University of Michigan-Dearborn, and the University of Vermont. Prior to joining the faculty at the Virginia Military Institute in the fall of 2004, Dr. Sullivan was employed by JMAR Inc. where he was involved in research and development of next generation lithography systems for the semiconductor industry.