Interlacing Engineering Graphics in an Introductory Engineering Materials Course as Visualization Aid

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Abstract

In an introductory engineering materials course, the basics of engineering graphics were utilized to generate three-dimensional models of crystals and molecules. AutoCAD™ software allowed the students to construct crystallographic models, while it helped them visualize the three-dimensional characteristics of different ceramic compounds. In order to build the computer models, the students were required to provide the geometrical features of each crystal. Specifically, they were required to provide the distances between atom centers, lattice parameters, atomic radii, and ionic radii, which helped them familiarize with the particularities of crystal structures of ionic, covalent and metallic solids. A student survey helped determine their perception of this crystal structure learning technique compared with the construction of foam ball models.

1. Introduction

In basic engineering materials courses, visual teaching tools have become a necessity to enhance the instruction [1]. Particularly useful are visualization techniques provided as slides [2] or in electronic format (CD-ROM, etc.) in the last generation of materials science and engineering textbooks [3]. These visualization software packages have become very popular, particularly when complex organic molecules are examined. In most cases those packages are available at a steep price while in few other cases they are free such as *Rasmol*.

On the other hand, in large class sizes it has been recommended the use of hands-on demonstrations as an alternative to full laboratory experiments [4]. For this purpose the students can be guided through a well-thought demonstration by teaching assistants. Alternatively, the present module proposes the use of computer graphics for a team assignment in a self-learning strategy to develop a three-dimensional perception of the structure of matter.

At the University of Puerto Rico – Mayagüez, as well as on other campuses, most engineering students in their fourth semester have already been trained in the use of computer graphics,

namely AutoCAD™. This fact allows the instructors of both the engineering graphics and the introductory engineering materials courses to design a team assignment to generate three-dimensional models of materials crystals and molecules. Succinctly, due to the students' familiarity with the graphics package, during the instruction of the materials science course, they were asked to generate models of assigned crystals and molecules. During lectures they were taught the essentials of atomic and molecular bonds, as well as the elemental unit cells and the structure of polymeric materials.

In due course, the proficiency in visualizing these structures help the instructor build upon that knowledge and facilitate the comprehension of physical and mechanical properties of the corresponding materials. This familiarity with in-depth structure-properties relationship is essential for materials as well as other engineers to develop criteria related to materials during their professional life. In modern industries, the concepts of materials science and engineering have become of significant importance [5].

2. Teaching Strategy

During the first week of classes students are organized in teams of four to five students to work on three team assignments throughout the semester. During the second week of instruction and after the students have familiarized with atomic and molecular bonding the concept of geometric arrangement of atoms in crystalline solids is introduced. The fourteen space or Bravais lattices and the corresponding six crystal systems are presented [6]. The symmetrical features of each unit cell are explained while the differences among Bravais lattices are clearly described based on angular and longitudinal dimensions: interaxial angles and lattice parameters.

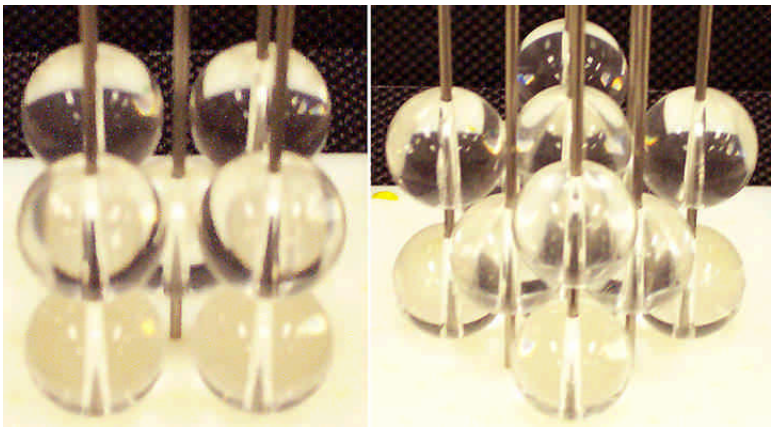
To generate this knowledge base (in the present case a full comprehension of the crystal and molecule geometry) related to evidence, the students need theory to provide a basis upon which to model the crystal or molecular structure. Moreover, graphical representations are considered concepts of evidence associated with data handling [7], which in the present teaching model is characterized by the relative position of atoms or ions in a crystal or molecule.

2.1 Metal Crystal Structures

To acquire a prompt appreciation of two basic cubic crystal structures common in most metals, the students are presented with foam models developed by prior student groups for a body-centered cubic (BCC) and face-centered cubic (FCC) unit cells (Figure 1 a and b, respectively) and the same unit cells constructed using a commercially available kit (Figure 2 and b). Immediately, during the instruction the students are asked to work in groups to determine the relation between the atomic radius r and the lattice parameter a (assuming a hard sphere model), namely: $4 \cdot r_{BCC} = \sqrt{3} \cdot a_{BCC}$ for a BCC metal and $4 \cdot r_{FCC} = \sqrt{2} \cdot a_{FCC}$ for an FCC metal. Then the students work on other basic characteristics of both unit cells, such as, the number of atoms included in each unit cell, the atomic packing factor, and a generic expression of the theoretical or volume density of different cubic metals.

(a) (b)

Figure 1: Foam ball models prepared by a prior group of students of this introductory course:
a) BCC unit cell
b) FCC unit cell



(a) (b)

Figure 2: Models constructed using the Solid-State Model Kit of the Institute for Chemical Education of the University of Wisconsin-Madison [8]:
c) BCC unit cell
d) FCC unit cell

2.2 Sodium Chloride and Cesium Chloride Crystal Structures

Ionic crystals are introduced next with the corresponding details on the ion sizes, and interionic distances. The simplest structures corresponding to NaCl and CsCl are given as examples of cubic unit cells. Other ionic and covalent (starting with diamond and silicon) solids follow through.

As it is well known, NaCl has a cubic closed-packed (rock salt) structure where the Cl^- anions are in an FCC arrangement and the Na^+ cations occupy all the octahedral sites having therefore octahedral coordination [9]. The centers of the Na^+ and Cl^- ions are located in the following lattice positions:

Na^+:	(½, 0, 0)	(0, ½, 0)	(0, 0, ½)	(½, ½, ½)
Cl^-:	(0, 0, 0)	(½, ½, 0)	(½, 0, ½)	(0, ½, ½)

With ionic radii equal to $r_{Na+} = 0.102$ nm and $r_{Cl-} = 0.181$ nm, the resulting lattice parameter is $a_{NaCl} = 2 \cdot r_{Na+} + 2 \cdot r_{Cl-} = 0.566$ nm

On the other hand, CsCl does not have a close-packed structure but a cell where Cl^- anions are located at the corners with the Cs^+ cations at the center of the body, or vice versa [10]. In this case the centers of the Cs^+ and Cl^- ions are located in the following coordinates:

Cs^+:	(½, ½, ½)			
Cl^-:	(0, 0, 0)	(1, 0, 0)	(0, 1, 0)	(0, 0, 1)

Coordination numbers are then for both ions equal to eight with the following ionic radii: $r_{Cs+} = 0.170$ nm and $r_{Cl-} = 0.181$ nm. From the relation between the lattice parameter and the ionic radii: $a_{CsCl} = 2 \cdot r_{Cs+} + 2 \cdot r_{Cl-} = 0.405$ nm.

2.3 Other Crystal Structures

Afterwards, two more ceramic cubic structures, zinc blende (ZnS) and perovskite, are presented and discussed. In particular, the $CaTiO_3$ is of interest since a perovskite-related structure will be assigned as part of a team project, as indicated in the following section. In the case of $CaTiO_3$ the positions of the center of the ions in the unit cell are as follows:

Ca^{2+}:	(0, 0, 0)	(1, 0, 0)	(1, 1, 0)	(0, 1, 0)
	(1, 1, 1)	(0, 1, 1)	(0, 0, 1)	(0, 1, 1)
Ti^{4+}:	(½, 0, 0)	(0, ½, 0)	(0, 0, ½)	(½, ½, ½)
O^{2-}:	(0, 0, 0)	(½, ½, 0)	(½, 0, ½)	(0, ½, ½)

Once the students have: a) acquired a knowledge basis and b) gone through a step-by-step example, they gain autonomy to begin working on a specific assignment. Explicitly, this assignment is to produce a rotating AutoCAD model of three different crystal structures:

- CsCl (following a step-by-step example)
- NaCl (first assignment)
- $BaTiO_3$ (second assignment)

3. AutoCAD™ Models

3.1. Example to Construct a Cesium Chloride CsCl (BCC) Crystal

During this first module step, the following detailed instructions were provided to the students to familiarize with the procedure. This was briefly preceded by a lecture with a worked example given in Section 2.2.

The instructions for the creation of a cesium chloride crystal are given in this paper exactly as they were given to the students so that any reader will be easily able to adopt this method of instruction in his/her own Materials Science class. Although the students at the University of Puerto Rico - Mayagüez already had sufficient experience using AutoCAD, the instructions are

stated simply enough so that even students (or instructors) without any prior experience using AutoCAD will be able to create 3D models in one class period.

1 Start AutoCAD

2 Create new file
`File → New → From Scratch`

3 Make sure coordinate arrows are on (check mark)
`Click: view → display → UCS icon → ✓ On`

4 Set color to red
`Click: arrow next to second white box in top menu → click: red`

5 Show shading
`Click: view (top menu) → shade → flat shaded or gouraud shaded`

6 Create center sphere (Specify center & diameter)
`Type: sphere [enter] → 0, 0, 0 [enter] → d [enter] → 0.181 [enter]`
`Type: zoom [enter] → E [enter]`

At this point the students have generated a sphere representing the central Cl^- anion of the CsCl crystal, as shown in Figure 3. They are ready to start graphing the eight Cs^+ cations with different colors. Due to central symmetry in this case it is convenient to locate the origin of coordinates at the center of the Cl^- ion; therefore, $\frac{a_{CsCl}}{2} = 0.101\text{nm}$.

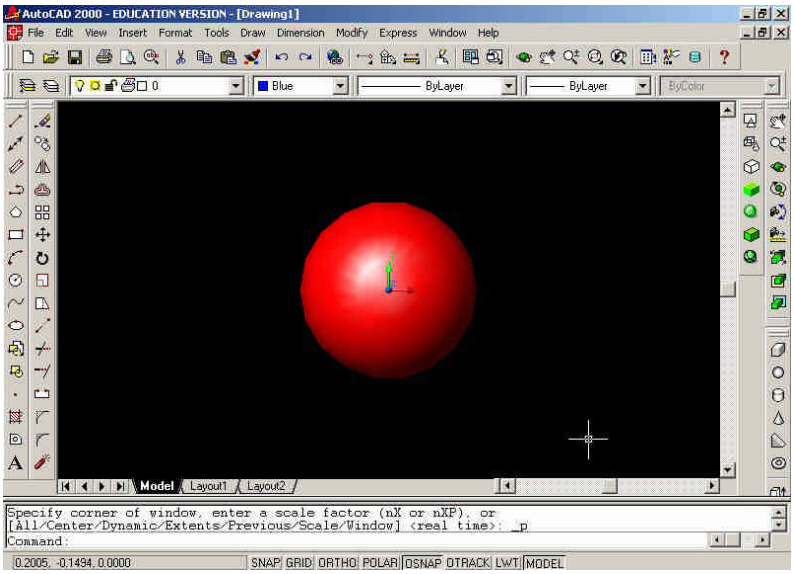


Figure 3: Initial step to generate the Cl- located in the center of the CsCl BCC crystal.

7 Change color
`Click: arrow next to second white box in top menu → click: blue`

8 Create first Cs^+ sphere

```
Type: sphere[enter] → -0.1010, -0.1010, -0.1010 [enter] → d [enter] →
      0.169 [enter] → zoom [enter] → E [enter]
```

The first cesium ion is located in the negative quadrant as shown in Figure 4.

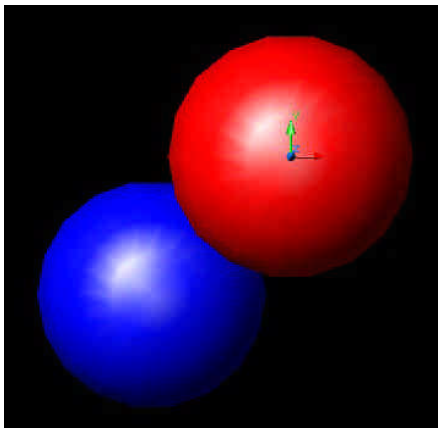


Figure 4: Construction of the first Cs+ cation located on one corner of the CsCl BCC crystal.

The following steps are a repetition of step 9 to locate the center of the Cs+ cations on the seven remaining corners of the crystal:

9 Locating the Cs+ cations

```
Repeat 8 using                -0.1010, 0.1010, -0.1010
Repeat 8 using                0.1010, 0.1010, -0.1010
Repeat 8 using                0.1010, -0.1010, -0.1010
Repeat 8 using                -0.1010, -0.1010, 0.1010
Repeat 8 using                -0.1010, 0.1010, 0.1010
Repeat 8 using                0.1010, 0.1010, 0.1010
Repeat 8 using                0.1010, -0.1010, 0.1010
```

10 Rotating object

```
Click: view → 3D orbit → click mouse anywhere on green line and move
```

Figure 5 displays the final CsCl model after the students start the rotation to enhance the perception of the 3-dimension structure.

There is an alternative way of drawing the cesium ions by using AutoCAD arrays. For this purpose one needs to follow instructions 1 through 8 to create the central chlorine ion as in Figure 3. If 0.169 nm is the calculated distance between the center of the chlorine and cesium atoms, then the corner spheres (Cs^+) are created as follows:

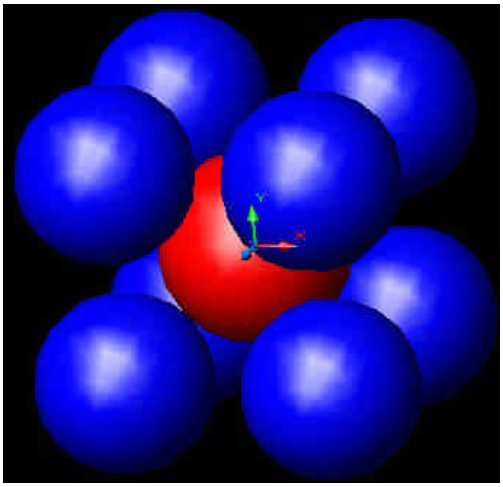


Figure 5: Final CsCl crystal where Cl^- is represented in red and Cs^+, in blue.

9' Create cesium spheres.

```
Sphere[enter] → -0.1010, 0.1010, -0.1010 [enter] → d [enter] → 0.169
[enter]
```

10' Create array.

```
Click: tool modify, array [enter] → sphere selection [enter] → R
[enter] → 2 [enter] → 2 [enter] → -0.202 [enter] → 0.202 [enter].
```

In this case the front layer of Cs^+ has been created, as displayed in Figure 6 where 0.202 nm is the calculated lattice parameter of CsCl. The crystal is completed as follows to generate a model identical to the one shown in Figure 5.

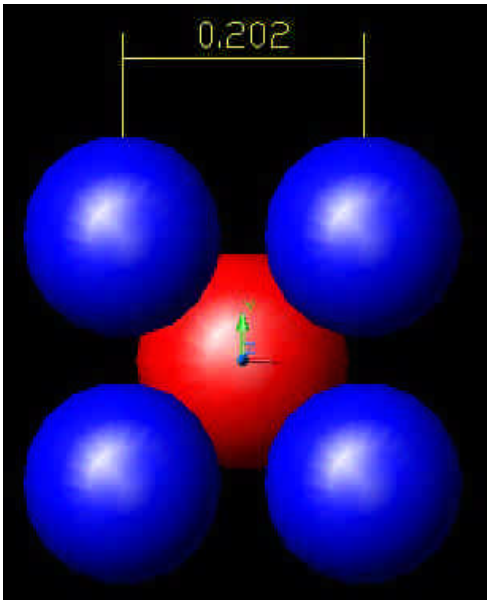


Figure 6: Creation of four Cs+ cations using arrays, displaying the CsCl lattice parameter.

To generate the other four cations and to view the rotating model the next steps should be completed:

14’ Copy array.
Click: copy → select the four spheres → paste in any place.

15’ Move the array.
Click: move → select the four spheres → select center of left superior sphere → -0.1010, 0.1010, 0.1010 [enter].

16’ Rotating object
Click: view → 3D orbit → click mouse anywhere on green line and move it.

Adding connecting bars that help visualize the cubic nature of CsCl results in a further enhancement of the crystal image:

17’ Create Connecting Bars. Note cylinders must always start on the x-y plane.
Choosing view → 3D view →Front, Top, Right, etc. will change global x, y, z coordinates

18’ Click: view . 3D view . front

i) Change color to green
ii) Type: cylinder → -0.1010, 0.1010, -0.1010 [enter] → 0.01 [enter] → 0.2020 [enter]
iii) Repeat ii) with -0.1010, -0.1010, -0.1010
0.1010, -0.1010, -0.1010
0.1010, 0.1010, -0.1010
iv) Click: view → 3D view → bottom
v) Repeat ii) and iii)
vi) Click: view →→3D view → right
vii) Repeat ii) and iii)

Before saving this work, a last check should be done by observing the front view to make sure the cubic crystal is apparent. This crystal can now be rotated to further appreciate the model and the connecting bars (Figure 7).

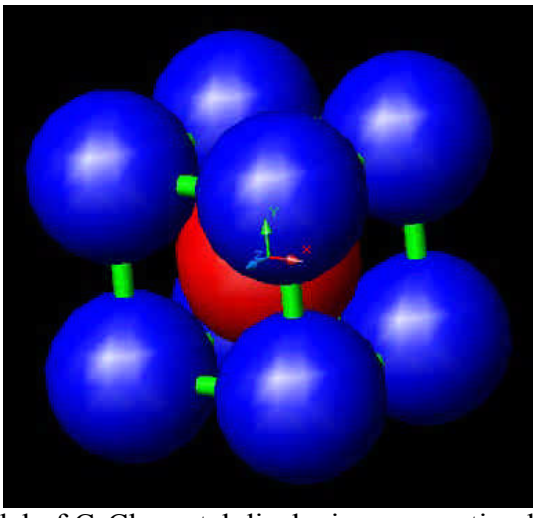
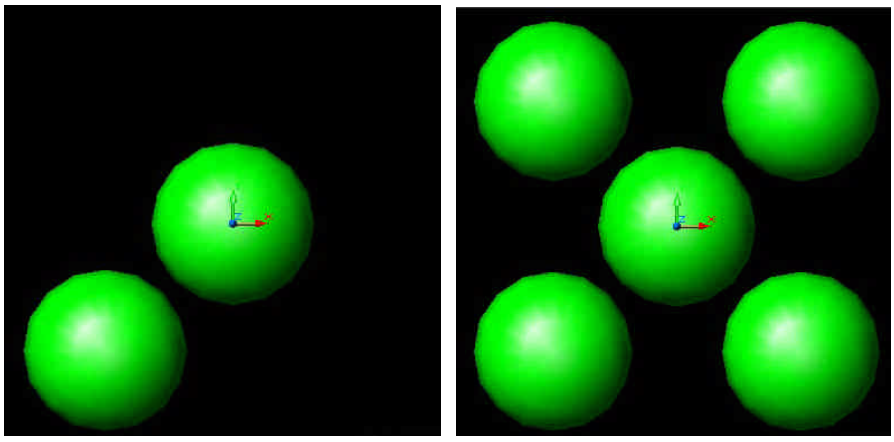


Figure 7: AutoCAD Model of CsCl crystal displaying connecting bars in this BCC unit cell.

3.2. First Assignment to Create a NaCl Crystal Model

For this first assignment the ion positions and lattice parameter computed in Section 2.2 are used. In this case, it is more convenient to locate the origin of coordinates at one Cl^- ion at the center of a face and then start drawing the other chlorine ions of that same face (Figure 8).

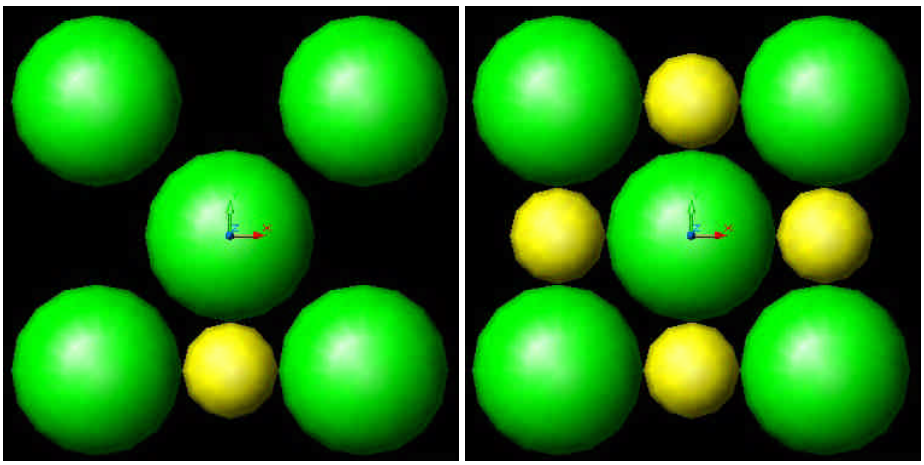
At half of the lattice parameter in the negative z axis, the first Na^+ is drawn in Figure 9 a, and this step is repeated for the other three sodium ions pertaining to that same face (Figure 9 b).



(a) (b)

Figure 8: Initial steps to build a NaCl crystal by using: a) chlorine ion at the center of a face as the origin and b) the remaining anions on the same plane.

For convenience the second layer of Cl^- anions is drawn in a negative quadrant. Although in this case the crystal is constructed in negative quadrants, it can also be reproduced in positive quadrants without major modifications (in fact this can be a comprehension test for this teaching module). Figure 9 a shows the first Cl^- drawn whereas in Figure 9b the whole layer is completed and the lattice parameter is also displayed. Finally, Figure 10 illustrates the finalized model after rotation.



(a) (b)

Figure 9: Location of: a) the first Na+ cation and b) the remaining three Na+.

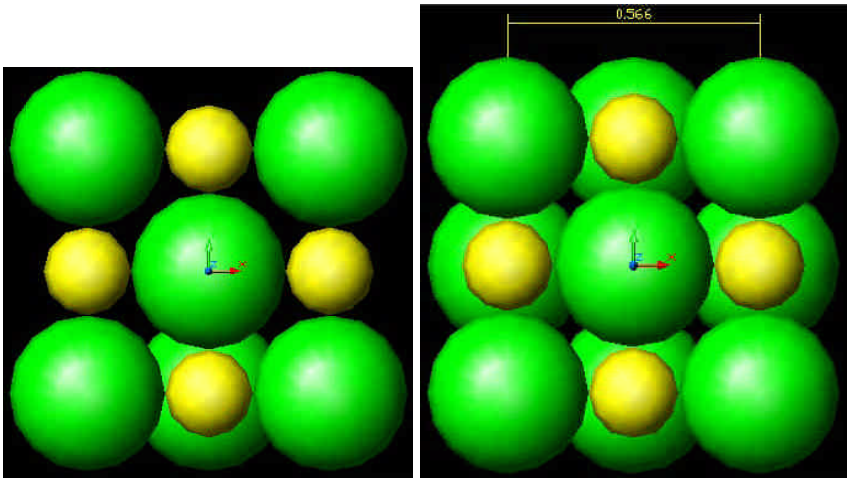


Figure 10: Drawing of second layer of four Cl^- anions:
a) First anion.
b) All four anions and lattice parameter indicated (0.566nm).

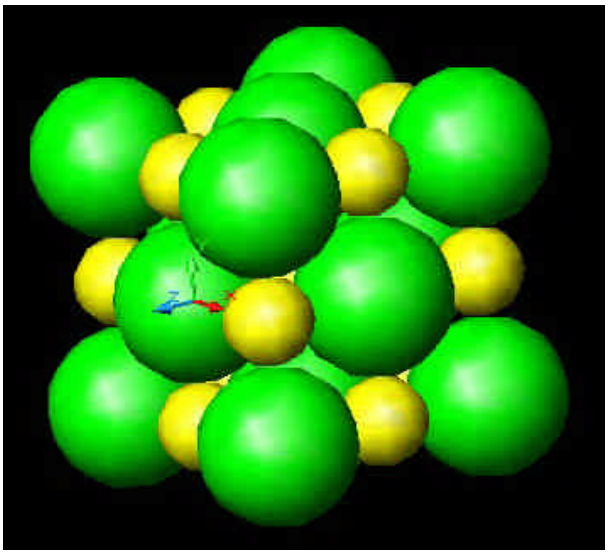


Figure 11: Final version of a NaCl crystal.

3.3. Second Assignment: Research the $BaTiO_3$ Crystal and its Piezoelectrical Property

$BaTiO_3$ is a typical piezoelectric material, i.e. under applied pressure this ionic insulator develops a voltage across its structure. Piezoelectricity, which is a reversible phenomenon, then results as a consequence of a change in the crystal dipole moment as the crystal is distorted [11]. On the unit cell vertical axis, there is a shift of Ti^{4+} cations of +0.006 nm, whereas the Ba^{2+} cations move down -0.009nm along the same axis [12].

For this second assignment the students were asked to construct a polarized (tetragonal) $BaTiO_3$ crystal indicating the radios of all ions, as well as the lattice parameters and to use different colors for different ions. With the pretext of presenting this polarized crystal structure in AutoCAD the students were additionally asked to search for information on piezoelectric materials.

For convenience in this case the origin is located at the center of a horizontal plane of the crystal. Then a Ba^{2+} cation is created as indicated in Figure 12.

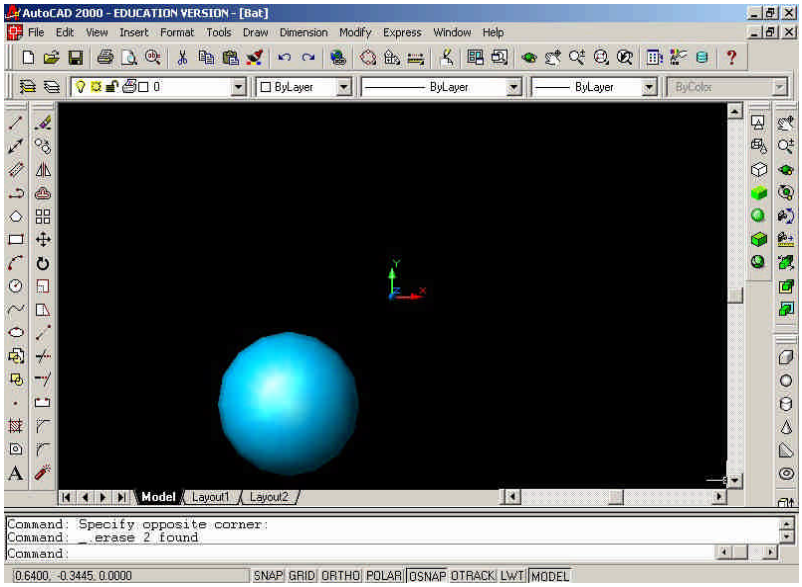
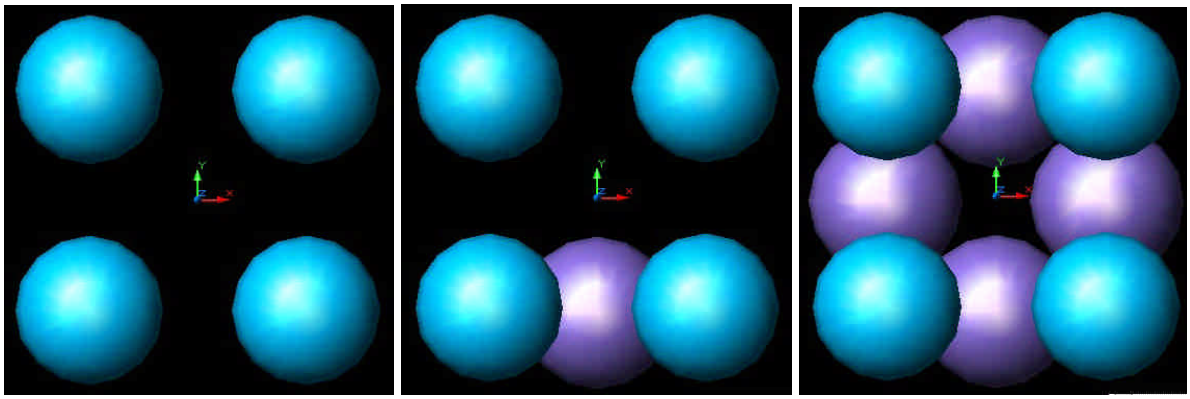


Figure 12: Initial step to create a $BaTiO_3$ crystal starting with a barium cation.

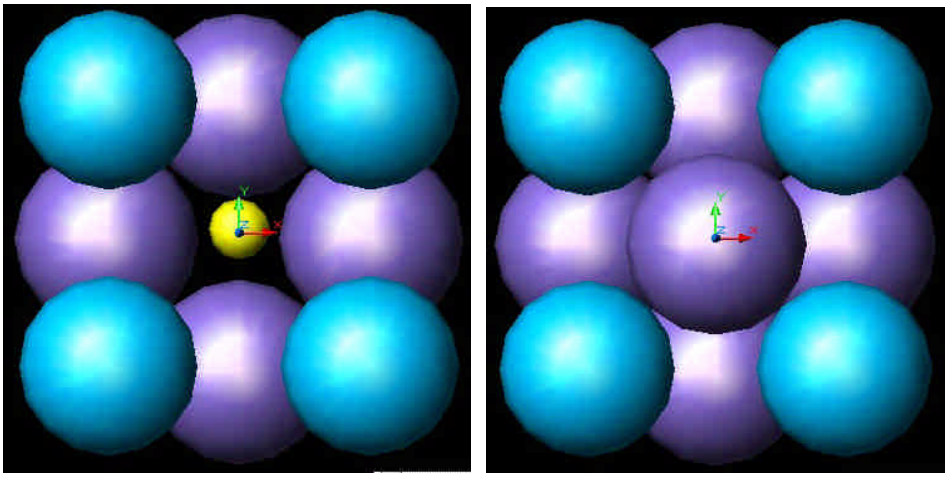
Figure 13 a through c illustrates the following steps. It should be noted that, due to the crystal polarization, the two upper Ba^{2+} ions are raised 0.009nm with respect to the plane containing the uppermost O^{2-} anion (Figure 13 c). This shift will become evident in a later image.



(a) (b) (c)

Figure 13: Subsequent steps involving:
a) First barium cation layer.
b) Generation of a O^{2-} anion
c) Completion of the oxygen anion layer.

The only Ti^{4+} ion of the crystal occupies an octahedral site formed by all the O^{2-} ions (Figure 14 a and b). However, because of the polarization, that cation is shifted 0.006nm on the vertical axis (Figure 14 a).



(a) (b)

Figure 14: Completion of two ion layers showing:

a) Drawing of the Ti^{4+} cation in the central octahedral site but displaced 0.006nm to indicate the polarization of the dielectric crystal.

b) Off-centric location of an O^{2-} anion.

To clearly demonstrate the polarization (and corresponding ion shifting), the AutoCAD sketch of Figure 15 is presented. All the corresponding distances including lattice parameters and distortions are indicated. Finally, the complete crystal is rotated and displayed in Figure 16.

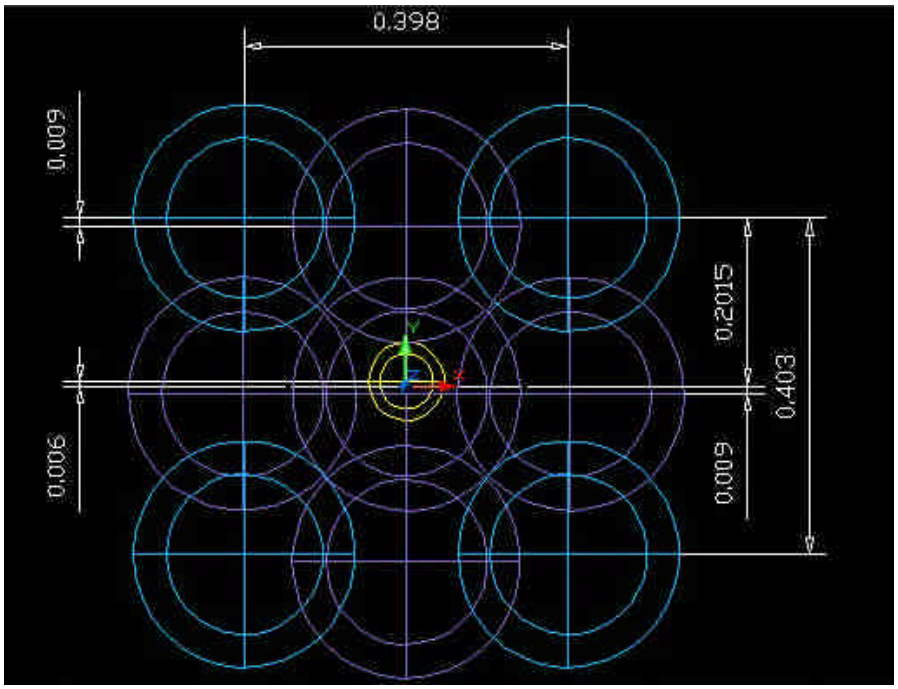


Figure 15: Sketch of the actual distances between ion centers drawn in Figure 1.

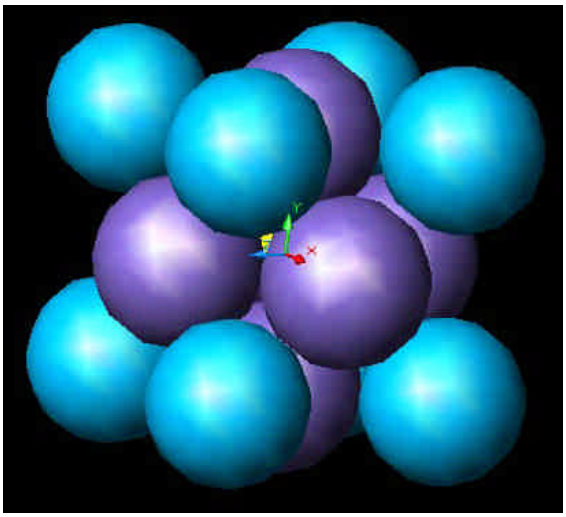


Figure 16: Final version of the polarized $BaTiO_3$ crystal structure where Ba^{2+} cations are represented as light blue spheres; the O^{2-} anions, as purple spheres; and, barely visible, the Ti^{4+} cation, as a yellow sphere in the octahedral site formed by the O^{2+} anions.

Further readings and Web searches on piezoelectricity bolster the understanding of the influence of crystal geometry on this property for a given dielectric material. Afterwards, a short discussion on dipole moment can help clarify the concept of piezoelectricity.

4. Assessment of the Instruction Effectiveness

4.1. Students' Survey Elements

After the completion of the assignment, the instructor carried out a survey of the students' opinion about using AutoCAD as a crystal-modeling tool. The number of students surveyed was 95. The following six statements were posed with two possible answers: a) Yes, I agree, or b) No, I disagree with the statement.

i. You suspect that constructing the models in AutoCAD was harder than using foam balls.
ii. After using AutoCAD you have a very good idea of the crystal geometry.
iii. You learned better the geometric arrangement by using AutoCAD.
iv. You had to be more careful with the actual dimensions by using AutoCAD.
v. As a future engineer you prefer to work with engineering tools, such as AutoCAD.
vi. You learned a little bit more about AutoCAD.

4.2. Analysis of Survey Results

The pie charts in Figure 17 a through f present the results of the survey. Although the students were not required to build foam ball models like those in Figure 1 a and b, a majority presume that such physical representation or construction could have been easier (Figure 17 a).

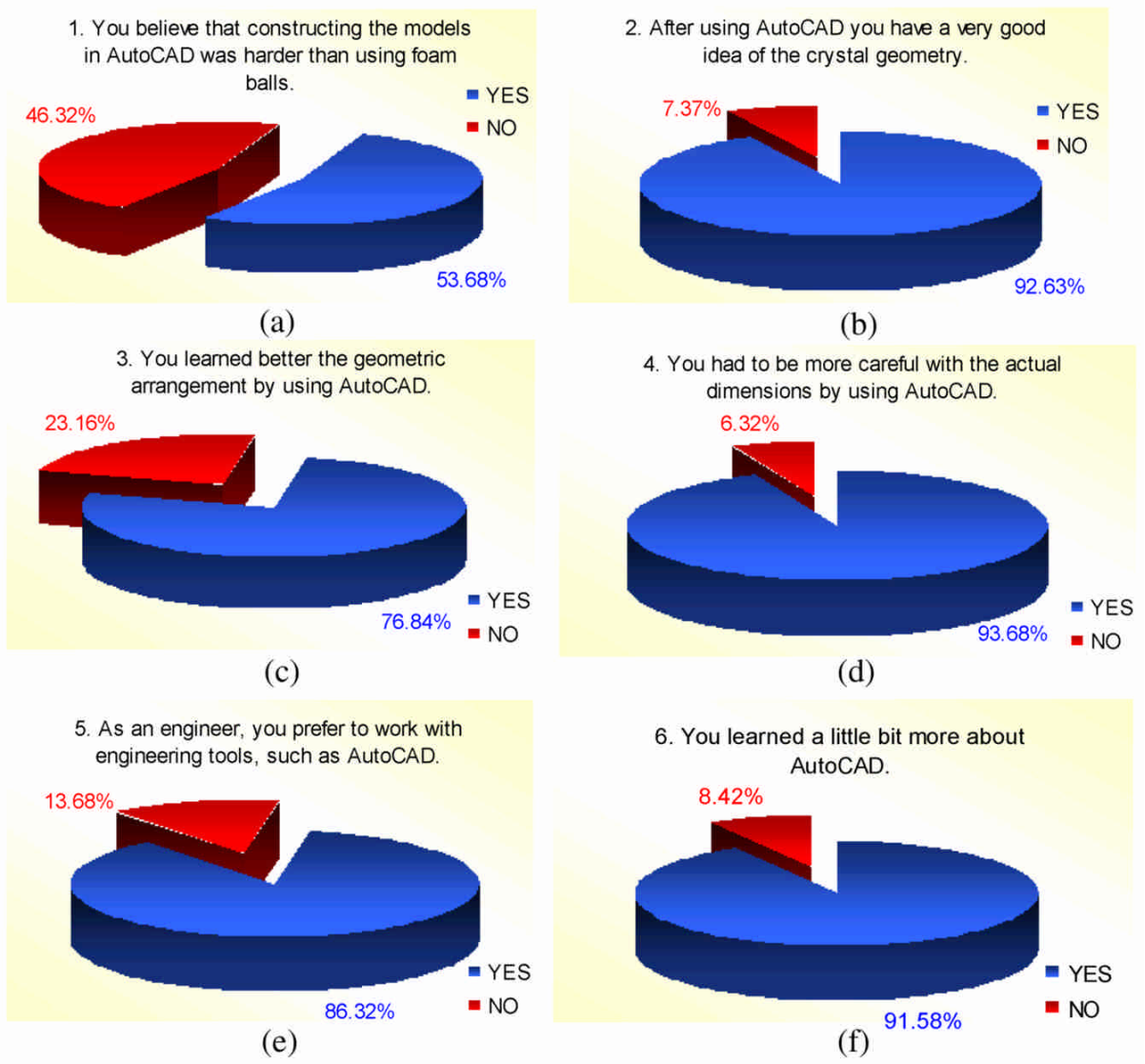


Figure 17: Pie charts of the results of the students' survey.

On the other hand, they realize how AutoCAD helps them comprehend the crystal geometry (Figure 17 b and c). Individual comments also indicate that before having to work on the tetragonal $BaTiO_3$ structure, they have not had a clear perception of the ion shifts that produced the polarization. These last two questions (ii and iii) were purposefully similar to detect any lack of precision in the students' answers. This could be explained by further students' comments point out that they have related statement ii) to the use of arrays in the construct, and that they have found this alternative somewhat harder.

The students are aware that with this graphic tool they have had to be meticulous in the dimensions of the crystals (Figure 17 d). As future engineers they know how important it is to develop special skills such as the use of AutoCAD (Figure 17 e and f). This is a particularly important conclusion since, except for those majoring in Civil and Mechanical Engineering, other students will not have further exposure in their undergraduate studies to this engineering graphics tool.

Because of those interesting findings the survey has proved to be very helpful and enlightening. As a consequence, the results encourage the instructor to keep using this technique as a visualization tool for the study of crystal geometry.

5. Summary

Although the use of experimental settings to teach materials behavior [13] continues to be essential in materials science and engineering, alternative and inexpensive methods are available to the instructor. In addition, the present teaching module presents a step-by-step method to construct three dimensional models using AutoCAD so that both instructor and students with minimal or no experience in this engineering graphics tool can reproduce the procedures. This methodical approach translates into a workshop which is enjoyable by the students and not time demanding.

In this respect the present teaching module details how engineering graphics tools can be implemented in the enrichment of a preparatory materials engineering course. Crystal and molecular structures are clear-cut examples of 3-D models that can be represented on a 2-D display (on paper or on a computer screen). Nevertheless, it should be remarked that this module was possible by reason of the particular curricula of the engineering programs at the University of Puerto Rico-Mayagüez. In effect, all engineering students at this university are required to take basic engineering graphics courses in their very first college years. Therefore, they are already familiar with AutoCAD when they register for the introductory course on engineering materials, which has as pre-requisites basic Physics and Chemistry courses. This is one of the advantages of five-year programs, which prepare versatile professionals with a solid background formation, as noted by a recent ABET accreditation visit to this campus. Students' opinions concur since they are aware that any additional skill learned represents an edge for their eventual job search.

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Biographical Information

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