

TEACHER INSTRUCTIONS

The Building Blocks of Ceramics

Objective: To introduce the concept of atomic ordering in crystal structures and demonstrate how different structures produce vastly different material properties.

Background Information: Many important material properties, such as strength, conductivity, and transparency, are highly dependent on how the atoms that make up that material are arranged and how those atoms interact with each other. These geometric arrangements of atoms are known as the *atomic* or *crystal structure*. Scientists and engineers have classified all of the possible atomic arrangements by geometric category, and the smallest possible group of atoms that maintain that shape are called *unit cells*. When these ordered unit cells are repeated over long distances, that material is classified as *crystalline*. When a material has no unit cell that can be repeated to describe its atomic ordering, it is classified as *amorphous*. Figure 1 shows representations of different geometric arrangements of common every day materials: table salt (sodium chloride), pencil "lead" (graphite), and window glass (silica). If you saw these materials at a scale 100,000 times smaller than the width of one human hair, this is what they would look like. For table salt and pencil lead, you can see a repeat unit cell, but for window glass, there is no long range order.



Figure 1: Representations of the atomic structures of table salt (a), pencil lead (b), and window glass (c).

a. <u>http://nersp.osg.ufl.edu/~wsawyer/atoms/chapter4/chapter4.html</u>

b. http://www.chemhume.co.uk/ASCHEM/Unit%201/Ch3IMF/Chemical%20Struct.html

c. Characterizing the hierarchical structures of bioactive sol-gel silicate glass and hybrid scaffolds for bone regeneration

R. A. Martin, et al. Phil. Trans. R. Soc. A 2012 370 1422-1443.

The structure that any given material has is dependent on many things, including the charge and size of the atoms that compose the material and the types of bonding taking place between those atoms. There are three types of primary atomic bonding: covalent, ionic and metallic bonds, and one major type of secondary bonding: Van der Waals (VDW) bonds. Each bond type has a relative energy, which can be



related to its strength. Engineers and scientists often model these bonds as springs with different stiffnesses. Table I shows the different bond types with associated bond energies as well as material examples.

Bond Type	Bond Energies	Materials
Covalent	120-1230 kJ/mol	Diamond, Silicon Carbide
Ionic	600-1500 kJ/mol	Sodium Chloride
Metallic	60-850 kJ/mol	Steel, Aluminum
Van der Waals	5-35 kJ/mol	Water molecules

The impact that different atomic bonding can have on materials is readily evident in everyday life. Common graphite and diamond are a great example because although both are made of the same element, carbon, they have very different properties (these are called *allotropes*). Diamond is the hardest material known to man, while graphite is one of the weakest. This discrepancy is due to the different structures of the two materials, which can be seen in Figure 2. Carbon atoms in diamonds are tightly bound in network covalent bonds. On the other hand, carbon atoms in graphite are only tightly bound by covalent bonds within the highlighted planes (shown in yellow in Figure 2) while VDW bonds weakly hold these planes together, meaning that they can shear apart easily. This property is why graphite is used as pencil 'lead'.



Figure 2. The atomic structure of diamond (left) and graphite (right), where each gray sphere represents a carbon atom. (Bodner Research Web of the Purdue Division of Chemistry Education).

The differences in bonding and structure also give rise to the discrepancy in optical and electrical properties between the two materials. Diamond is transparent and is a good electrical insulator, while graphite is black in color and is often used as an electrode in energy applications because it conducts electrons well.

Lab Description: In this lab, various crystal unit cells will be constructed using toothpicks, springs, foam spheres, and twist ties. The students can be broken into groups and will work together to first construct different unit cells with foam spheres connected by tooth picks, as shown in Figure 3. They will then construct some of those same unit cells with springs to demonstrate the difference in the strengths of



different crystal structures. Students will be asked to make predictions about the properties of the resulting crystals based on these unit cell models.



Figure 3: A basic structure, simple cubic, to be built during the student activity portion of this lesson.

Keywords:

- \cdot crystal structure: unique arrangement of atoms in a crystal.
- \cdot unit cell: the simplest repeating arrangement of atoms in a crystal.
- crystalline: structure that exhibits long range ordering; atoms are arranged in repeating patterns.
- \cdot amorphous: exhibits no long range ordering of atoms.
- \cdot allotropes: materials that are made of the same element but that have different structures.

Materials List (supplies needed per group):

- · 15 small foam spheres (packing peanuts can be used as a cheap alternative)
- · 40 toothpicks
- \cdot 20 small springs (to avoid buying a lot, the students can take turns using that work station to use them)
- \cdot 16 twist ties

Safety Precautions: Standard lab rules and procedures should be followed (only using the equipment as indicated in the instructions). Toothpicks are sharp and present a hazard.

Instructions:

Simple cubic model

- 1. Gather 8 foam spheres, 12 tooth picks, and 12 small springs.
- 2. On a flat surface, create a square with 4 spheres and 4 tooth picks.
- 3. Repeat with the remaining 4 spheres.
- 4. Lay the square from step 2 flat and pierce each sphere vertically with a toothpick.
- 5. Form a cube by fixing the second square from step 3 onto the top portion of the tooth picks.
- 6. The final simple cubic structure model should look like this (Figure 4):





Figure 4: Schematic of simple cubic model.

- 7. Next replace the toothpicks in the cubic structure model one by one with springs.
- 8. Push one corner of the cubic structure lightly, and record your observations of the structure's ability to withstand the force you applied (how much does it deform, does it appear sturdy?).

Body- centered cubic model

- 1. Collect 1 more sphere and 8 more springs.
- 2. Take the cubic structure you just made (connected by springs) and now place one sphere ball in the center of that cube, and connect it using 8 more springs to each of the 8 corners of the cube. You have now created a body centered cubic structure (Figure 5).
- 3. Push one corner of the body center cubic model structure, and record your observations of the structure's ability to withstand the force you applied.
- 4. Disassemble the structure.



Figure 5: Schematic of a body-centered cubic

Face-centered cubic (FCC) model

- 1. Gather 14 foam spheres and 36 tooth picks.
- 2. Repeat steps 2-6 of the simple cubic model.



3. On each face of the resulting cube, use 4 toothpicks to attach one sphere at the center of each face, as shown in Figure 6.



Figure 6: Schematic of the construction of one face of the face centered cubic model.

4. A schematic drawing of the final face centered cubic model structure is shown below in Figure 7.



Figure 7: Schematic of the face centered cubic model.

Fluorite structure model

- 1. Collect 1 more foam sphere, 4 more tooth picks, and 16 twist ties.
- 2. With one sphere and 4 toothpicks, construct the following tetrahedral structure:



Figure 8: Schematic (left) and model made of zip ties (right) showing the tetrahedral structure.

For simplicity, this structure can be represented using twist ties, as shown above in Figure 8.

- Collect 2 twist ties, and fold both in half. With the zip ties folded in half, crease them to make a V shape. Each V shaped twist tie should be approximately ¹/₄ as tall as your cubic structure. You can also cut the zip ties to make them the correct length.
- Twist the two V shaped twist ties together so that the Vs are facing opposite diagonals and one is pointing down while the other is pointing up, as pictured.



3. Insert the tetrahedral structure into your face centered cubic structure as shown in Figure 9.



Figure 9: Schematic showing the location of a tetrahedral structure in the face centered cubic

You can remove a couple of the connecting toothpicks to make it easier to insert the tetrahedral structure.

4. Now imagine 7 more tetrahedral structures being incorporated into the structure as shown in Figure 10 (if time permits, students may continue to construct the remaining tetrahedral structures to include in the structure).



Figure 10: Schematic the location of all tetrahedral structures in the fluorite showina structure.

5. Complete the questions on the Student Question Handout.

Computational tool to help visualize:

If computer access is available, you can also have students use an open source computational tool called nanoHUB that will allow them to run their own simulations to create 3D renderings of these structures. It can be found here: <u>https://nanohub.org/resources/crystal_viewer</u>

- 1. Open the link to the nanoHUB site.
- 2. Select the "Launch Tool" button (blue, found on the right, middle of the page). You will have to make a login to use the tool. There is also a first time user guide located under the "Launch Tool" button if you would like to explore more ways to use nanoHUB.



- 3. Click "Settings" at the bottom right.
- 4. Select I want to... "view a material" from the pull down menu.
- 5. Select a structure from the pull down menu next to "Choose a crystal structure:". Several crystal structures talked about in this lesson are available for simulation, such as diamond, face centered cubic, body centered cubic, and sodium chloride.
- 6. Click the "Simulate" button at the bottom right to create the 3D rendering of that structure. The structure can be rotated to help in visualization.

Clean Up:

- 1. Taking precaution with the sharp toothpicks, disassemble all models.
- 2. Place all materials in their designated storage containers, as instructed by your teacher.
- 3. Wipe down surfaces that have any particle residue from foam spheres.



TEACHER DISCUSSION QUESTIONS

The Building Blocks of Ceramics

Discussion Questions to Ask Before the Lab

1. Looking at the structure of graphite, ask students how they think that structure is oriented on the tip of their pencil (if they could look at the tip of their pencil and see the atoms)? Why? If it were oriented differently, do they think they would still be able to write with it?

Discussion: Remind them that bonding in graphite is strongest along certain planes. The reason they can see their writing on the page is because the lead is oriented such that the yellow planes in Figure 2 are parallel to the page. That way when they write, the weakest bonds in graphite are broken by the force of their hand and the material in the strongly bonded planes is left on the page to show up as letters, lines, etc. If it were oriented otherwise, the force of their hands wouldn't be able to break the strong bonds within those planes, and no writing would show up.

2. Ask students if they can think of any other materials that are both made of the same element, but have vastly different properties (like the diamond vs. graphite example).

Discussion: Oxygen is a common allotrope. One structure is gaseous O_2 , which you breathe in through the air, and another is O_3 , or ozone, commonly found in the Earth's atmosphere. A second illustration is the difference between quartz and glass, allotropes of SiO₂. Sand is made of crystalline quartz, while window glass is made of amorphous SiO₂.

Discussion Question to Ask After the Lab

You can discuss question 5 in the student handout further as well as the extra credit questions, and use the information about ceramics in fuel cells included in the supplementary info.

Discussion: The structure model referred to in question 5 is the fluorite structure, and the material is cubic zirconia. Further uses of zirconia are electrolytes for solid oxide fuel cells and oxygen sensors next to the catalytic converter in car exhausts. Another engineering material that adopts the fluorite structure is uranium dioxide, commonly used as nuclear fuel.





SUPPLEMENTARY INFORMATION

http://mypages.iit.edu/~smart/garrear/fuelcells.htm

A fuel cell is a device that generates electricity by a chemical reaction. Every fuel cell has two electrodes, one positive (cathode) and one negative (anode). The reactions that produce electricity take place at the electrodes. Every fuel cell also has an electrolyte, often a version of zirconia, which carries electrically charged particles from one electrode to the other, and a catalyst, which speeds the reactions at the electrodes. The purpose of a fuel cell is to produce an electrical current that can be directed outside the cell to do work, such as powering an electric motor or illuminating a light bulb, or a city. Because of the way electricity behaves, this current returns to the fuel cell, completing an electrical circuit.



STUDENT LAB HANDOUT

The Building Blocks of Ceramics

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Table I. Examples of bond types, energies, and example materials.

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Keywords: crystal structure, unit cell, crystalline, amorphous, allotropes



Materials List:

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Figure 3: Schematic of simple cubic model.

- 7. Next replace the toothpicks in the cubic structure model one by one with springs.
- 8. Push one corner of the cubic structure lightly, and record your observations of the structure's ability to withstand the force you applied (how much does it deform, does it appear sturdy?).

Body-centered cubic model

1. Collect 1 more sphere and 8 more springs.



2. Take the cubic structure you just made (connected by springs) and now place one sphere ball in the center of that cube, and connect it using 8 more springs to each of the 8 corners of the cube. You have now created a body centered cubic structure (Figure 4).



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- 3. Insert the tetrahedral structure into your face centered cubic structure as shown in Figure 8. You can remove a couple of the connecting toothpicks to make it easier to insert the tetrahedral structure.



Figure 8: Schematic showing the location of a tetrahedral structure in the face centered cubic



4. Now imagine 7 more tetrahedral structures being incorporated into the structure as shown in Figure 9 (if time permits or your teacher instructs you to do so, continue to construct the remaining tetrahedral structures to include in the structure).



Figure 9: Schematic showing the location of all tetrahedral structures in the fluorite structure.

5. Complete the questions on the Student Question Handout.

Clean Up:

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- \cdot Place all materials in their designated storage containers, as instructed by your teacher.
- \cdot Wipe down surfaces that have any particle residue from foam spheres.



STUDENT QUESTION HANDOUT

Building Blocks of Ceramics

1. What observations did you make after performing step 8 on the simple cubic model?

2. What observations did you make after performing step 3 on the body centered cubic model? How did this compare with the deformation seen with the simple cubic structure? If you were going to build a material that needed to be easily deformed, which would you use?

3. If the face centered cubic and fluorite structure models were both made with springs connecting all of the spheres, which would you assume will be strongest (most resistant to deformation)? Why?

4. One of the structure models you made is the basic building block of one of the most widely used engineering ceramics. This material is known for its high hardness and ability to withstand harsh environments. It is used for a wide range of applications: for dental implants because of its hardness, and in jet engines for its ability to withstand high temperatures (3 times as hot as your oven at home!) and corrosive environments – to name a couple. Which of these structure models do you think it is?



*Extra Credit

1. What material do you think is referred to in question 5?

2. Based on what you have learned about bonding and material properties, how do you think bond energy relates to strength (i.e., if you have something with high bond energy, do you think it has high strength)?

3. How do you think bond strength relates to melting point? Would diamond or graphite have a higher melting temperature, and why?



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