

Unit Cells and Crystal Structures



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Based on a work at www.nano-link.org

Unit Cells and Crystal Structures

Abstract

In this module students create a saturated solution using borax, sodium acetate, and copper sulfate. Upon drying, each crystal will have a different shape. The shape at the macro level is driven by the arrangement of atoms. This repeating arrangement of atoms is the defining characteristic of a crystal structure, and is based on the geometry of the fundamental unit cell. Students may introduce other chemicals to change the resulting structure. This module serves as a good introduction to crystal structures supplementing the typical ball and stick models.

Outcomes

Student will gain a basic understanding of crystal structures and their properties, and how crystals form.

Prerequisites

Students should have some exposure to the following physical science concepts typically encountered in eighth grade science:

- The basic understanding of atoms
- The basics of chemical bonds

Correlation

Science Concepts

- Atomic nature of solid materials
- Structure of crystalline materials
- Crystal unit cells

Nanoscience Concepts

- Forces and interactions at the nanoscale--ionic and covalent bonding
- Properties of materials

Background Information

A crystal (or crystalline solid) is a material whose constituent atoms, molecules, or ions are arranged in an orderly repeating pattern extending in all three spatial dimensions. The scientific study of crystals and crystal formation is known as crystallography. The process of crystal formation is called crystallization or solidification. The word crystal is derived from the ancient Greek word κρύσταλλος (krustallos), meaning both “ice” and “rock crystal”, [1] from κρύος (kruos), “icy cold, frost”. [2] [3] Examples of crystalline solids include water ice, minerals such as quartz and halite (rock salt), and many gem stones, such as rubies and diamonds. Most common metals, including gold, silver, iron, and copper, have a crystalline microstructure consisting of many tiny crystalline regions; this type of solid is called polycrystalline.

Crystal structure

Crystallization is the process of forming a crystalline structure from a melt liquid or from materials dissolved in a liquid. For example, water when cooled undergoes a phase change from the liquid to its solid form (ice). During the phase change, the water molecules are initially in the disordered state of the liquid. As they cool and lose thermal energy, the molecules begin to line up in the ordered crystalline arrangement found in ice. The orderly crystal represents a lower energy state than that of the disordered liquid, so this phase change releases some energy, known as the heat of fusion, into the surrounding environment.

In most cases during freezing, many small crystals will form simultaneously and then grow until they fuse, forming a polycrystalline structure. Under the right circumstances, one large crystal can be made to grow into a macroscopically large sample. These so-called single crystal materials are important in many fields of technology.

The physical properties of a crystalline solid depend on the size and arrangement of the individual crystals, or grains. Which crystal structure the fluid will form depends on the chemistry of the fluid, the conditions under which it is being solidified, and on the ambient pressure. While the cooling process usually results in the generation of a crystalline material, under certain conditions, the fluid may be frozen in a noncrystalline state. In most cases, this involves cooling the fluid so rapidly that atoms cannot travel to their lattice sites before they lose mobility. A noncrystalline material, which has no long-range order, is called an amorphous, vitreous, or glassy material. It is also often referred to as an amorphous solid, although there are distinct differences between crystalline solids and amorphous solids: most notably, the process of forming a glass does not release the latent heat of fusion.

Crystalline structures occur in all classes of materials, with all types of chemical bonds. Almost all metals exist in a polycrystalline state; amorphous or single-crystal metals must be produced synthetically, often with great difficulty. Ionically bonded crystals, such as salts like sodium chloride and potassium chloride, can form upon solidification of the salts, either from a molten fluid or upon crystallization from a solution. Covalently bonded crystals are also very common, notable examples being diamond, silica, and graphite.

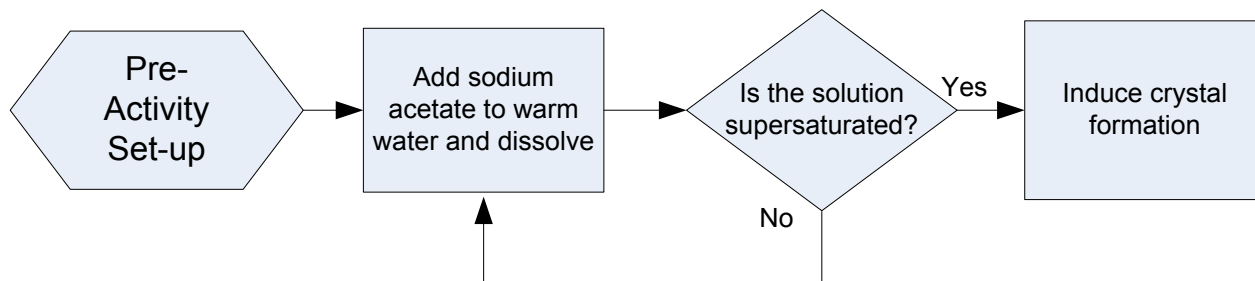
Polymorphism is the ability of a solid to exist in more than one crystal form. For example, water ice is ordinarily found in the hexagonal form designated ice Ih, but can also exist with cubic crystals (ice Ic), the rhombohedral ice II, and many other forms. Amorphous phases are also possible with the same molecule, such as amorphous ice. In this case, the phenomenon is known as polyamorphism. For pure chemical elements, polymorphism is known as allotropy. For example, diamond, graphite, and fullerenes are different allotropes of carbon.

While the term "crystal" has a precise meaning within materials science and solid-state physics, colloquially "crystal" refers to solid objects that exhibit well-defined and often pleasing geometric shapes. In this sense of the word, many types of crystals are found in nature. The shape of these crystals is dependent on the types of molecular bonds between the atoms to determine the structure, as well as on the conditions under which they formed. Snowflakes, diamonds, and table salt are common examples of crystals. Some crystalline materials may exhibit special electrical properties such as the ferroelectric effect or the piezoelectric effect. Additionally, light passing through a crystal is often refracted or bent in different directions, producing an array of colors; crystal optics is the study of these effects. In periodic dielectric structures a range of unique optical properties can be expected as seen in photonic crystals.

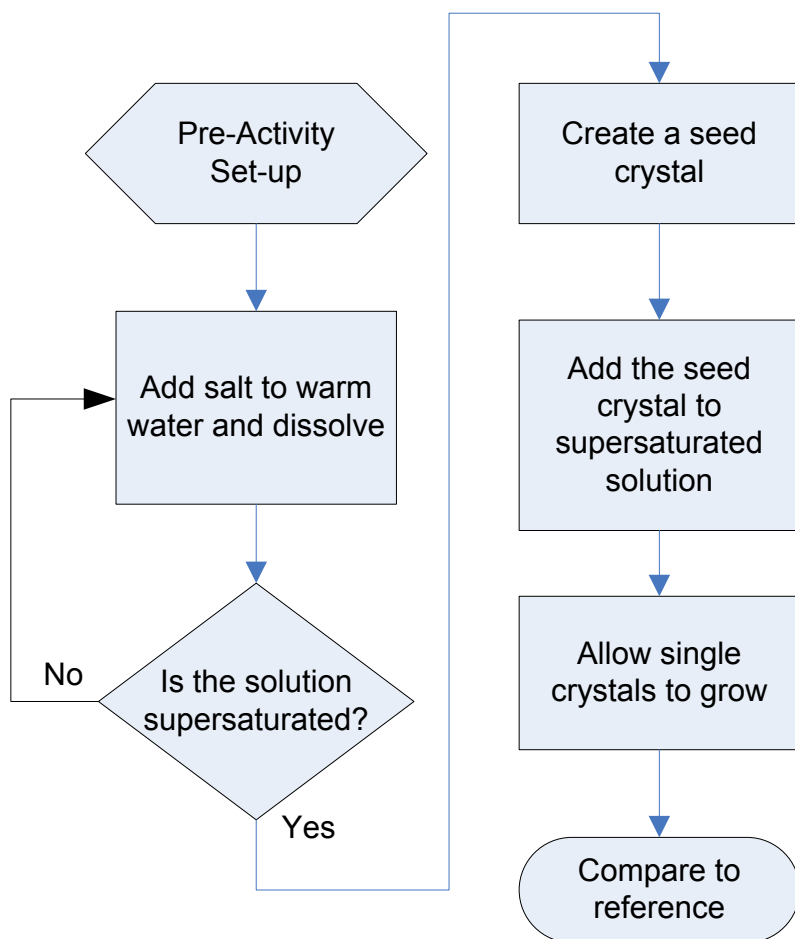
Learning Activity

Activity Flow Chart

Part 1. Making a Super Saturated Solution



Part 2. Growing crystals



Learning Activity

I. Making a Super Saturated Solution

Background. A super saturated solution is a solution that has more substance dissolved in it than it could normally hold at room temperature. In this activity you will create super saturated solutions and then grow crystals from these solutions.

Materials

- Distilled or deionized water
- Sodium acetate, anhydrous
- Test tube and test tube rack
- Hotplate and beaker or water bath
- Plastic or glass Petri dishes
- Stir sticks

Procedure

1. Fill a test tube with water to a height of 2 cm from the bottom of the tube.
2. Add enough sodium acetate powder so the total height of the water plus the powder is 3 cm from the bottom of the tube.
3. Stir in the sodium acetate until fully dissolved making sure to scrape the bottom
4. Add more sodium acetate until you can't dissolve any more into the solution, again, making sure to scrape the bottom.
5. Put the test tube into a water bath and heat the solution until all the powder has dissolved and the solution is clear. DO NOT BOIL.
6. Once the sodium acetate is fully dissolved, remove the test tube from the water bath and pour a small amount into a petri dish, then set GENTLY into a test tube rack to cool down (5-10 minutes).
7. Once the solution has cooled, agitate the solution by flicking or tapping the test tube and watch the crystals grow. If flicking or tapping doesn't work, then you can drop 1 sodium acetate crystal (seed crystal) into the solution. It may take a couple minutes to notice the crystals forming.

Note: During the first 2 steps it is very important that you continue to add the sodium acetate until you truly can't dissolve anymore. The dissolving process takes a little while. If you stop stirring too soon, it is possible the solution will not be supersaturated and the experiment won't work.

II. Growing Crystals Activity

Materials

- Plastic or glass beakers
- Distilled or deionized water
- Material for crystallization. Possibilities include
 - Borax (sodium borate)
 - sodium acetate
 - copper sulfate
- Pencil and thread

Procedure

1. Label beakers. *NOTE:* Larger volumes of water will require more material to reach saturation. Final volumes (step 4 below) only require a depth of two centimeters.
2. Saturate solutions
 - a. Prepare solutions of the salts you are using by first dissolving the materials in warm water, stirring frequently.
 - b. Continue to add material until you observe undissolved solid collecting in the bottom of the beaker.
 - c. Once the solution is super saturated, allow it to cool.
3. Collect a seed crystal to grow a larger single crystal sample
 - a. Dip a length of thread into the saturated solution
 - b. Allow the thread to dry
 - c. Remove any excess crystals
4. Pour the saturated solution into two separate beakers to at least a depth of two centimeters.
5. Set up the crystal growth chamber
 - a. Suspend the thread made in Step 3 from a pencil laid across the top of the jar.
 - b. Place beaker in desired conditions (i.e., ice bath, fridge, countertop) undisturbed.
6. Monitor crystal growth, which may take a few hours to a few days.
7. Research the type of material used in the experiment, determine the expected crystal structure, and find some images of these crystals.
8. Examine the crystals you grew, using a hand lens magnifier and/or an optical microscope. Make a sketch of the crystal shapes below. Compare your crystals to the results found in Step 7.

Discussion Questions

1. What do the following terms mean?
 - a. super saturated
 - b. amorphous material
 - c. polycrystalline
 - d. exothermic/endothemic
 - e. crystal defects
 - f. grain boundary
2. Briefly discuss your experience with crystal growth in this activity.
3. Where else do you see crystals?
4. Why do we need to know the crystal structure of a material? Explain (in a general sense) how different structures can result in different properties.
5. What types of defects may have been introduced in the crystals you grew?
6. What environmental aspects of your experiment may have contributed to what you observed?
7. Was the crystal growth endothermic or exothermic? Why?
8. What are some practical uses for a super-saturated solution of sodium acetate?
(Think of the chemical hand warmers used for cold weather outdoor activities.)
9. How is this experiment an example of self -assembly?

Questions 10-16 assume that the instructor has gone over the PowerPoint slides with the class, covering material on crystal form and unit cell terminology.

10. What is a unit cell?

11. The lengths of the unit cell sides, usually designated as a , b and c , are most often measured in what units?
12. How many atoms per unit cell are there in a body centered cubic (BCC) crystal structure?
13. For a BCC unit cell what do $(1,0,0)$, $(1,1,0)$, $(1,1,1)$ and $(0,0,1)$ represent?
14. Draw a ball and stick BCC unit cell.
15. For the unit cell shown in Figure 1,
 - a. Label x , y and z axes.
 - b. Since this is a cubic structure, and the length of each side is the same, call that value " a ".
 - c. Show these " a " dimensions on your unit cell drawing.
 - d. Draw the directional vector (index) corresponding to $[110]$.
 - e. Write the algebraic equation you would use to determine the length of the vector you drew in #7. Use " x " as the length of this directional vector.
 - f. Solve the above algebraic equation for " x ".

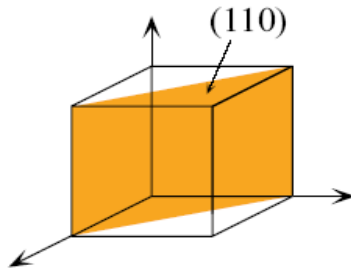


Figure 1. Unit cell.

16. What type of unit cell does the sodium acetate crystal exhibit?

Current and Future Applications

Crystals and crystal growth are very important in many areas of science and engineering. Virtually all integrated circuits are made using a substrate of single crystal silicon and use layers of polycrystalline materials. Managing crystal growth is essential in producing steel and other metals, where the crystal structure determines metal strength, ductility, and other properties. Crystalline materials are also used in optical and optoelectronic devices.

Understanding crystal growth is also important to the earth sciences. In geophysics, minerals in the Earth's crust grow from the melt to form various types of igneous rock. In meteorology, the growth of ice crystals plays a central role in understanding cloud dynamics, lightning, and the formation of rain and hail.

Contributors

This activity was originally developed by Kristie Jean of the North Dakota State College of Science. It was edited and modified by Deb Newberry of Dakota County Technical College and James Marti of the University of Minnesota.

Multimedia Resources

Videos

- Super saturated solutions
- http://www.youtube.com/watch?v=1y3bKIOkcmk&feature=player_embedded

Simulations

- www.nanohub.org
- www.concord.org

Articles

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Additional References

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3. The American Heritage Dictionary of the English Language, Fourth Edition: Appendix I: Indo-European Roots. 2000.
4. National Geographic, 2008. Cavern of Crystal Giants (<http://ngm.nationalgeographic.com/2008/11/crystal-giants/shear-text>).

Alignment of Unit Cells and Crystal Structures Module to the Next Generation Science Standards

- The Next Generation Science Standards (NGSS) were published in April 2013. They consist of statements that convey the performance expectations for students. Each performance expectation is a single statement that is built from three parts: science and engineering practices (Practices), disciplinary core ideas (DCI) and crosscutting concepts.

The background material, reading, and the slides from the module address the aspects of the NGSS shown in Table 1.

TABLE 1. ALIGNED PRACTICES, DISCIPLINARY CORE IDEAS, AND CROSSCUTTING CONCEPTS

| PRACTICE | DCI | CROSSCUTTING CONCEPT |
|--|---|---|
| <p><i>MS Analyzing and Interpreting Data:</i> Analyze and interpret data to determine similarities and differences in findings.</p> <p><i>Partial in student materials</i></p> | <p><i>MS.PS1-A:</i> Solids may be formed from molecules, or they may be extended structures with repeating subunits (e.g., crystals).</p> <p><i>Strong in teacher and student materials</i></p> | <p><i>MS Structure and Function:</i> Structures can be designed to serve particular functions by taking into account properties of different materials, and how materials can be shaped and used.</p> <p><i>Strong in teacher and student materials</i></p> |

Alignment of Unit Cells and Crystal Structures Module to the Common Core State Standards in English Language Arts/Literacy and Mathematics

The Common Core State Standards (CCSS) were published in June 2010. They articulate student skills for English language arts/literacy and mathematics. The content of the module addresses the concepts and skills shown in Tables 3 and 4.

For English language arts/literacy, the CCSS is organized around College and Career Anchor Standards (CCR) that articulate the over-arching skills that students need to be prepared for college and career. There are grade level versions of each Anchor Standard, as well as versions for science and social studies classrooms (literacy standards). Alignments in Table 3 were made to the Anchor Standards, unless a more specific version of the standard was a closer fit to the skills in the module. Additional alignments may be warranted, depending on the use of associated videos that are provided as links in the module and whether students engage in discussions.

TABLE 3. ALIGNED COMMON CORE STANDARDS FOR ENGLISH LANGUAGE ARTS & LITERACY

CCR.L.6: Acquire and use accurately a range of general academic and domain-specific words and phrases sufficient for reading, writing, speaking, and listening at the college and career readiness level; demonstrate independence in gathering vocabulary knowledge when encountering an unknown term important to comprehension or expression.

Partial in teacher and student materials

CCR.W.7: Conduct short as well as more sustained research projects based on focused questions, demonstrating understanding of the subject under investigation.

Partial in student materials

For mathematics, Table 4 shows alignments to standards found in the 8th through 12th grade levels.

TABLE 4. ALIGNED COMMON CORE STANDARDS FOR MATHEMATICS

No alignments