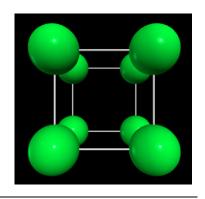
# <u>Crystal Lattice Structure Solids & 3D Printing Technology</u> USE THE GUI FILES

## A. Simple Cubic Structure Example

- 1. Open the file **Cubic Structure Example** by clicking on <a href="https://cs.boisestate.edu/~mlong/GUI/crystal">https://cs.boisestate.edu/~mlong/GUI/crystal</a> <a href="https://cs.boisestate.edu/~mlong/GUI/crystal">httml/po</a> obs.html
- 2. Click **Run** to see how the solid is rotated and **Pause** it to explore the rotation from different viewpoints.
- 3. Rotate: use Right Button Drag or Ctrl-drag
- 4. Zoom: Drag with the middle Button or use Scroll Wheel.
- 5. Click **Reset** to get it back to its original position.



#### **Vocabulary**

**Simple (or Primitive) Cubic Structure.** Polonium is a rare and highly radioactive metal. It has the simplest but also rare crystal structure called primitive cubic or the simple cubic denoted as "cP". This structure consists of the smallest repeating pattern of the cube with one lattice point on each corner of the cube.

**Parameter** is a numerical or measurable quantity whose value is selected for the particular circumstances and in relation to which other variable quantities may be expressed.

**Lattice constant a:** a standard **parameter** represents the distance between two atoms in units of Å (Anstrom,  $10^{-10}$ m).

Atomic/ionic radius: a parameter represents the radius of one atom or ion.

## Launch

Open the file **Cubic Structure Example**.

- 3. There are 8 atoms in this solid, do they have a fixed distance between the two consecutive atoms? Why or why not?

## **Explore**

Stay on the file **Simple Cubic Structure Example**.

Click **Run** to see how it is rotated and **Pause** it to explore the rotation from different viewpoints.
Provide two pictures of the solid from two different viewpoints.

2. Try to **Rotate** the solid, use **Right Button Drag** or **Ctrl-drag**. What type(s) of symmetry does it have?

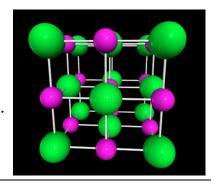
#### 3. The lattice constant a:

- What is the parameter of the lattice constant a for this cubic cell? (Provide a value and a unit)
- Change the parameter of the **lattice constant a** to half of its initial value. Provide a picture of the new image.
- Change the parameter of the **lattice constant a** to double its initial value. Provide a picture of the new image.

## B. Face-centered Cubic (fcc) Structure

**NaCl is the chemical symbol for Sodium Chloride** that occurs naturally as white crystals of salt. It consists of two types of ions: positive sodium ions (symbol: Na+) and negative chloride ions (symbol: Cl-) which alternate with each other in each of the three dimensions.

- 1. Open the website **NaCl** by clicking on <a href="https://cs.boisestate.edu/~mlong/GUI/crvstal">https://cs.boisestate.edu/~mlong/GUI/crvstal</a> html/nacl v1 obs.html
- 2. Click **Run** to see how the cell of NaCl is rotated and **Pause** it to explore the rotation from different viewpoints.
- 3. Rotate: use Right Button Drag or Ctrl-drag
- 4. Zoom: Drag with the middle Button or use Scroll Wheel.
- 5. Click **Reset** to get it back to its original position.



#### **Vocabulary**

**Face-centered Cubic** crystal structure has a repeating pattern of lattice in the shape of cube, and there are also lattice points on the **centers** of **faces** of the cube.

ra: ionic radius of component A (such as Na+ in this case).

**rb:** ionic radius of component B (such as Cl- in this case).

### Launch

Open the website NaCl.

- 1. Focus on the structure of NaCl, describe its shape
- 2. What is the measurement unit used in describing the size of Na+ and Cl-?
- 3. Describe how Sodium (Na+) and Chloride (Cl-) ions are related in terms of their radius and volume. Show your work.

4. What is the parameter of **the lattice constant a** for bonded structure of Na+ and Cl-, and what does it mean? 5. What is the number ratio between Na+ and Cl-? **Explore** Stay on the website NaCl. 1. Click **Run** to see how the fcc structure of NaCl is rotated and **Pause** it to explore the rotation from different viewpoints. Provide two pictures of it from two different viewpoints. 2. Try to Rotate the fcc structure of NaCl, use Right Button Drag or Ctrl-drag. What type(s) of symmetry does it have? 3. Compare the fcc structure of NaCl in A. Cubic Structure Example and the fcc structure of <u>NaCl</u> in **NaCl**. Discuss the structure and types of symmetry they have. 4. Parameter of the lattice constant a. What is the parameter of the lattice constant a for NaCl? (make sure to include the unit) \_\_\_\_\_ Change the parameter of the **lattice constant a** to half of its initial value. Provide a

picture of the new image.

• Change the parameter of the **lattice constant a** to double its initial value. Provide a picture of the new image.

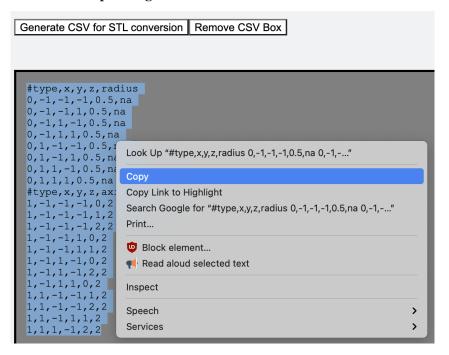
5. Change the parameters **ra** and **rb three** times but **keep the lattice constant a fixed** (5.64), explore the differences. In the table below, document the changes and provide an image of NaCl in each case.

ra	rb	ra	rb	ra	rb

6. We can design 3 new fcc materials by changing all of those parameters (**ra**, **rb and a**), let's explore the differences. In the table below, document the changes and provide an image of new in each case.

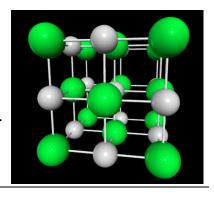
lattice constant a =		lattice constant a =		lattice constant a =	
ra	rb	ra	rb	ra	rb

- 1. Explore possible fcc structures using the provided app and click the button at the bottom of the page.
- 2. Save the content from the output window in your email. This is the file we are going to use for 3D printing. We recommend to keep L=1. A larger number of atoms means longer printing and waiting time is needed for printing.



## **Extension**

- 1. Open the website **AgCl** by clicking on <a href="https://cs.boisestate.edu/~mlong/GUI/crystal">https://cs.boisestate.edu/~mlong/GUI/crystal</a> html/agcl v1 obs.html
- 2. Click **Run** to see how the cell of NaCl is rotated and **Pause** it to explore the rotation from different viewpoints.
- 3. Rotate: use Right Button Drag or Ctrl-drag
- 4. Zoom: Drag with the middle Button or use Scroll Wheel.
- 5. Click **Reset** to get it back to its original position.



## **Review STEM Concepts**

Use your own language to explain the following concepts:

#### • Math

- a. Polygon (2D)
- b. Polyhedron and Platonic solids (3D)
- c. Measurement
- d. Coordinates
- e. Symmetry
- f. Ratio
- g. Similarity

#### • Materials Science

- a. Atoms
- b. Crystal Structures
- c. Crystalline

### • Computer Science

- a. Class
- b. Object
- c. Attribute