Crystal Lattice Structure Solids & 3D Printing Technology

C. Body Centered Cubic (bcc) Lattice Structure

Iron is known as α-iron or ferrite below 912 °C (1,674 °F). It has a body-centered cubic (bcc) crystal structure. This structure consists of the smallest repeating pattern of the cube with one lattice point on each corner of the cube and one at the center of the cube (body).

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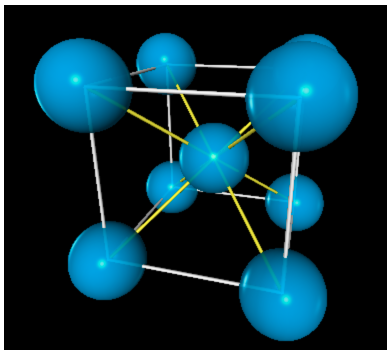
1. Open the file **Fe (metal iron)** by clicking on https://cs.boisestate.edu/~mlong/GUI/crystal_html/fe_obs.html
2. Click **Run** to see how the fcc structure of NaCl is rotated and **Pause** it to explore the rotation from different viewpoints.
3. **Rotate:** use **Right Button Drag** or **Ctrl-drag**
4. **Zoom: Drag with the middle Button** or use **Scroll Wheel**
5. Click **Reset** to get it back to its original position.



Open the file **Fe (metal iron).**

1. Focus on the structure Fe, describe its shape

   _____

2. Describe how Iron (Fe) atoms are related in terms of their radius, surface area and volume. Show your work.

Explore

Stay on the file **Fe (metal iron).**

1. Click **Run** to see how the **Fe** is rotated and **Pause** it to explore the rotation from different viewpoints. Try to **Rotate** the **Fe (metal iron)**, use **Right Button Drag** or **Ctrl-drag.** Provide two pictures of it from two different viewpoints.

2. What type(s) of symmetry does it have?

3. Compare NaCl in **B. Cubic Structure Example (FCC sturcture in Part 1)** and **Fe (metal iron, BCC structure).** 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** of **Fe (metal iron)**?

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   - 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.

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D. 3D Representation of Ideal Perovskite Lattice Structure

A **Perovskite** is a colorless mineral of **Calcium Titanate** with the chemical formula **CaTiO3.** It was discovered by German mineralogist Gustave Rose who named it after a Russian mineralogist Lev Alexeievitch Perovskite. Later, perovskites are referred to a family of materials with the same crystal structure as **CaTiO3.** So the general chemical formula for this category of perovskite compounds is **ABX3**, where A is a metal cation (positively charged ion), B is a cation and X is an anion (negatively charged ion). If X is oxygen, the sub-category can also be represented as **ABO3. CaTiO3** consists of three types of ions: positive Calcium ions (symbol: Ca+), Titanium ions (symbol: Ti+) and negative Oxygen ions (symbol: O-) which alternate with each other in each of the three dimensions. In a unit cell, Ca+ occupies the corners, Ti+ occupies the center of the lattice and O- are at the center of faces.

Similarly, **SrTiO3 (Strontium Titanate)** consists of three types of ions: positive Strontium ions (symbol: Sr+), Titanium ions (symbol: Ti+) and negative Oxygen ions (symbol: O-) in the same way. It is one of the few materials with ideal perovskite structure (no slight distortion).

Perovskites are of great importance in material science and can be widely applied to photovoltaics, laser.

Perovskite solar cells: Solar cells with **perovskite structures** have shown remarkable progress in improving energy conversion efficiency, from reports of about 3% in 2006 to over 24% in 2019 and thus are thought to be a frontier energy solution. The Department of Energy is of great interest in research to increase the efficiency and lifetime of hybrid organic-inorganic perovskite solar cells.

There are two GUI files for Ideal Perovskite Structure solids. One for **Calcium Titanate (CaTiO3)**, and one for **Strontium Titanate (SrTiO3)**

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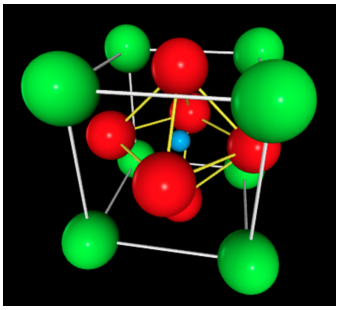
1. Open the file **SrTiO3 (Strontium Titanate)** by clicking on https://cs.boisestate.edu/~mlong/GUI/crystal_html/srtio3_obs.html
2. Click **Run** to see how the fcc structure of NaCl is rotated and **Pause** it to explore the rotation from different viewpoints.
3. **Rotate:** use **Right Button Drag** 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

Crystal structure: a description of the highly ordered arrangement of atoms or ions in crystals.

a: A standard lattice parameter presenting the distance between 2 neighboring Sr+ ions.

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

rb: ionic radius of component B (such as Ti+ in this case).

ro: ionic radius of component C (such as O- in this case).

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Launch

Open the file **SrTiO3 (Strontium Titanate).**

3. Focus on the structure of SrTiO3, describe its shape

   _____

4. Describe how Strontium (Sr+),Titanium (Ti+) and Oxygen (O-) ions are related in terms of their radius, surface area and volume. Show your work.

Explore

Stay on the file **SrTiO3 (Strontium Titanate).**

5. Click **Run** to see how the SrTiO3 is rotated and **Pause** it to explore the rotation from different viewpoints. Provide two pictures of it from two different viewpoints.

6. Try to **Rotate** the SrTiO3, use **Right Button Drag** or **Ctrl-drag.** What type(s) of symmetry does it have?

7. Compare NaCl in **B. Cubic Structure Example (FCC sturcture in Part 1)** and **SrTiO3 (Strontium Titanate, perovskite structure).** Discuss the structure and types of symmetry they have.

8. Parameter of the **lattice constant a.**
   - What is the parameter of the **lattice constant a** of Sr+, Ti+ and O-?

     _____

   - 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.

9. Change the parameters **ra, rb** and **ro three** times but **keep the lattice constant fixed** (3.988), explore the differences. In the table below, document the changes and provide an image of "new" **perovskite** solid in each case.

ra	rb	ro	ra	rb	ro	ra	rb	ro

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

lattice constant a =			**lattice constant a** =			**lattice constant a** =		
ra	rb	ro	ra	rb	ro	ra	rb	ro

Review STEM Concepts

Use your own language to explain the following concepts:

- **Math**
  a. Polygon (2D):
     - A plane shape consisting of a finite number of line segments.
  b. Polyhedron and Platonic solids (3D):
     - (Regular) Tetrahedron has 4 triangular faces, with 3 meeting at each vertex, 6 straight edges, and 4 vertices.
     - Cube has 6 squares, with 3 meeting at each vertex, 12 straight edges and 8 vertices.
     - (Regular) Octahedron has 8 equilateral triangles, with 4 meeting at each vertex, 12 edges, and 6 vertices.
  c. Measurement
     - A comparison with a fixed reference amount of a quantity. The reference amount is called unit.
  d. Coordinates
     - A system using numbers (e.g., x, y, z) to determine positions of geometrical elements

e. Symmetry
   - Translation: A shape or design if there is a translation of the plane such that the design or pattern as a whole occupies the same place in the plan both before and after translation.
   - Rotation: A shape or a design in a plan, if there is a rotation of the plane of more than 0 degrees but less than 360 degrees, such that the shape or design as a whole occupies the same points in the plan both before and after rotation.
   - Reflection: A shape or a design in a plan, if there is a line in the plane such that there are matching parts when the shape or design is folded along the line. Coordinates

f. Ratio
   - Two quantities are in ratio A to B if there are N x A units of the first quantity, N x B units of the second quantity.

g. Similarity
   - Two objects are similar if every point on one object corresponds to a point on the other object and there is a positive K, such that the distance between any two points on the second object is K times as long as the distance between the corresponding points on the first object.
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- **Materials Science**

a. Atoms
   - An atom is the smallest unit of ordinary matter that forms a chemical element.

b. Crystal Structure
   - A description of the ordered arrangement of atoms, ions or molecules in a crystalline material

c. Crystalline
   - A material in which the atoms are situated in a repeating or parodic array

- **Computer Science**

a. Class
   - A user-defined type specifying attributes

b. Object
   - An instance or run-time entity of a class

c. Attribute
   - Properties of a class of objects