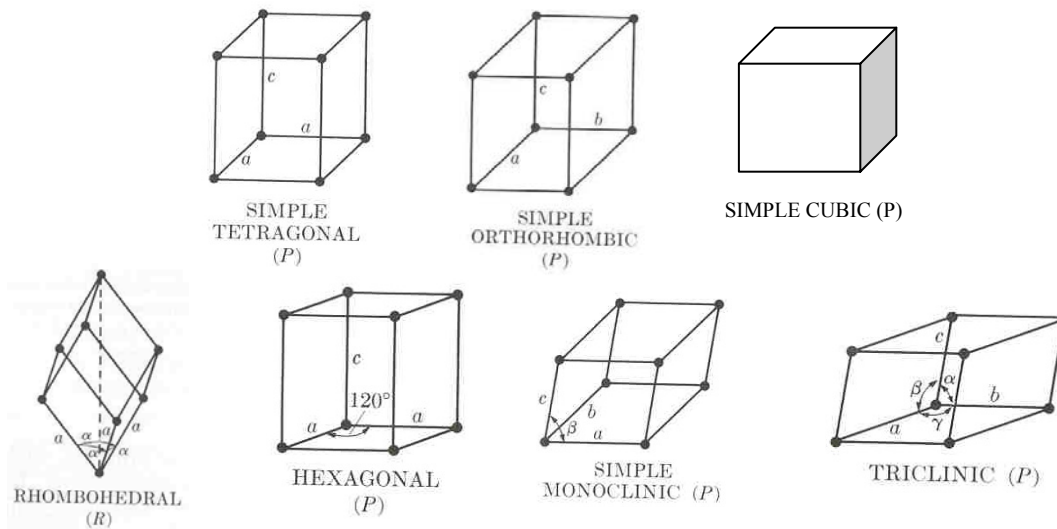


Go to "Student Learning Resources, Callister 6e", from the "Start" menu, "All Programs." Choose "Interactive MSE" from the pull-down menu. Click on the "Crystallography and Unit Cells" icon, choosing "Crystal Systems/Unit Cells."

**(1) Crystal Systems:** Take time to examine each of the seven crystal systems, using the rotation buttons on the left.

- (a) Cubic:  $a = b = c; \alpha = \beta = \gamma = 90^\circ$
- (b) Tetragonal:  $a = b \neq c; \alpha = \beta = \gamma = 90^\circ$
- (c) Orthorhombic:  $a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ$
- (d) Rhombohedral or Trigonal:  $a = b = c; \alpha = \beta = \gamma \neq 90^\circ$
- (e) Hexagonal:  $a = b \neq c; \alpha = \beta = 90^\circ; \gamma = 120^\circ$
- (f) Monoclinic:  $a \neq b \neq c; \alpha = \gamma = 90^\circ \neq \beta$
- (g) Triclinic:  $a \neq b \neq c; \alpha \neq \beta \neq \gamma \neq 90^\circ$



**(2) Atomic Coordinates:** Now take time to examine the body-centered cubic lattice (BCC) and the face-centered cubic lattice (FCC). Assume that the lattice parameter is a unit length of 1.

- (a) What are the coordinates of each of the atom positions in the simple cubic lattice?
- (b) What are the coordinates of each of the atom positions in the BCC lattice?
- (c) What are the coordinates of each of the atom positions in the FCC lattice?

**(3) Atoms/Unit Cell:** Take a look again at the simple cubic, BCC, and FCC lattices.

- (a) How many atoms belong to the simple cubic unit cell?
- (b) How many atoms belong to the BCC unit cell?
- (c) How many atoms belong to the FCC unit cell?

**(4) Comparison of Crystal Structures:** Now go to "Modules" and click on "Ceramic Structures."

- (a) Click on the CsCl molecule. The yellow ball is the cesium ion  $\text{Cs}^+$  and the blue ball is the chlorine ion  $\text{Cl}^-$ . How many ions are in this unit cell of CsCl?
- (b) What are ion positions for  $\text{Cs}^+$ ?
- (c) What are the ion positions for  $\text{Cl}^-$ ?
- (d) Is CsCl a BCC structure? Explain why or why not. If not, what structure is it?
- (e) Now click on the NaCl molecule. The blue ball is the  $\text{Na}^+$  and the yellow ball is the  $\text{Cl}^-$ .

- (f) What are the ion positions for  $\text{Na}^+$ ?
- (g) What are the ion positions for  $\text{Cl}^-$ ?
- (h) How many ions are in this unit cell of NaCl?
- (i) What kind of lattice structure is NaCl?
- (j) Now take a look at the ZnS structure, also called the zinc-blende structure. What type of lattice do the red balls (S) form?
- (k) Describe the atomic positions of the blue balls (Zn)? These positions are called tetrahedral sites because they form a tetrahedron in each corner of the unit cell.
- (l) Are all the tetrahedral sites filled in this unit cell? What is the maximum number of tetrahedral sites possible?
- (m) Now look at the diamond structure. What is the main difference between it and the ZnS structure?
- (n) Examine the fluorite structure ( $\text{CaF}_2$ ) by rotating it around. How would you describe this structure in terms of "body-centered," "face-centered," or "simple" atomic positions?
- (o) Now look at the barium titanate structure. Describe the atomic positions of each of the three different colored balls. Given that the molecular formula for barium titanate is  $\text{BaTiO}_3$  and that the radius for  $\text{Ti}^{4+}$  is 0.068 nm compared to  $\text{Ba}^{2+}$  0.136 nm (from your textbook), what color ball corresponds to what element?

**(5) Closed-Packedness: Stacking in Crystal Systems:** Now click on "Modules" again and go back to "Unit Cells – Crystal Systems."

- (a) Click on the HCP structure. HCP stands for hexagonal-close-packed, which illustrates how the atoms are stacked in this crystal lattice. The HCP lattice structure is common in metals. In an HCP metal, the atoms in the second layer are above the hollows in the first layer and the atoms in the third layer are above the atoms in the first layer, so that the layer stacking sequence can be summarized as A B A B A B ... Rotate the structure around so that you can see the A-B-A stacking.
- (b) Since the close-packedness is only somewhat obvious in the software, take a look at the Styrofoam balls to see how the atoms in the B layer fill into the hollows of the A layer, and the atoms of the A layer fill into the hollows of the B layer, ...
- (c) Close-packedness is also easy to see in cubic systems. Using the Styrofoam balls and the toothpicks, create a simple cubic lattice. Given the radius  $r$  of each atom, represent the lattice parameter  $a$  in terms of  $r$ .
- (d) Using the Styrofoam balls and the toothpicks, create a BCC lattice. Given the radius  $r$  of each atom, represent the lattice parameter  $a$  in terms of  $r$ .
- (e) Using the Styrofoam balls and the toothpicks, create an FCC lattice. Given the radius  $r$  of each atom, represent the lattice parameter  $a$  in terms of  $r$ .

**(6) Bonding and Properties of C-Based Structures:** Take a look again at the diamond structure and compare that to the HCP structure. We all know that diamond is itself a very hard, almost unbreakable material, but that graphite, which has the HCP structure, "writes well," or its bonds are easily broken. Both materials are made of carbon (C) atoms only and both materials are covalently bonded (with the bonding between the A-B layers being secondary pi-bonds in graphite). Looking at the bonding and the atomic structure of each material, explain why these properties make sense.