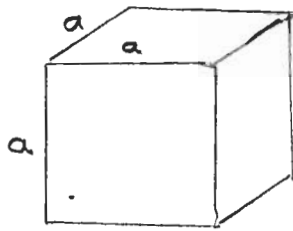


**Solid Modeling Module: Crystal Structures**

- A. Type of activity/investigation:** This module allows students to consider the atomic structures of crystals by constructing models with the atoms idealized as spheres. To begin this module, the teacher should have a large container filled with marbles. Students are asked to guess the number of marbles in the jar. The teacher then introduces the concept of crystal structures. The regular order and the close packing associated with crystalline materials in part explains the strength of these materials. Two basic structures, the body-centered cubic (BCC) and face-centered cubic (FCC) are presented. Students will then model these structures in SolidWorks. The teacher will then introduce the concepts of a unit cell and packing factor. By selectively cutting away portions of their models, the students construct unit cells – the building blocks of atomic structures. The SolidWorks program can calculate the volume of atoms within the unit cell cube. By ratioing this volume to the volume of a solid cube of the same size, the packing factor can be determined – 68% for BCC and 74% for FCC. The students are then asked to apply these results to their guesses as to the number of marbles in the jar. A discussion of estimation is appropriate here. The packing factor is based on ideal conditions. Are the marbles perfectly packed within the box? How much should we reduce the ideal packing factor to simulate the conditions of our real system?
- B. Engineering concepts investigated:** Materials science – effect of atomic structures on material properties.
- C. Mathematics concepts investigated/needed:** None for baseline module. Geometry and trigonometry for advanced options.
- D. Science concepts investigated/needed:** Chemistry – atomic structures
- E. Materials needed for the module:** SolidWorks
- F. Estimated time needed for the module:** 3 hours
- G. Educational Outcomes:**
1. Identify and model common crystal structures
  2. Calculate packing factors for crystal structures
- H. Techniques for instructional differentiation:**
- Advanced Students
1. Calculate packing factors by hand, using geometry (need to be able to find hypotenuse of a right triangle, volume of a sphere).
  2. Model the hexagonal close-packed (HCP) structure and its unit cell, find the packing factor with software.
  3. Find packing factor of HCP by hand (requires trigonometry of right triangles).
  4. Research to find materials with various crystal structures.

CALCULATION OF PACKING FACTORS:SIMPLE  
CUBIC:EACH ATOM HAS  
RADIUS  $r$ ATOMS ON ADJACENT CORNERS TOUCH, SO  $a = 2r$ 

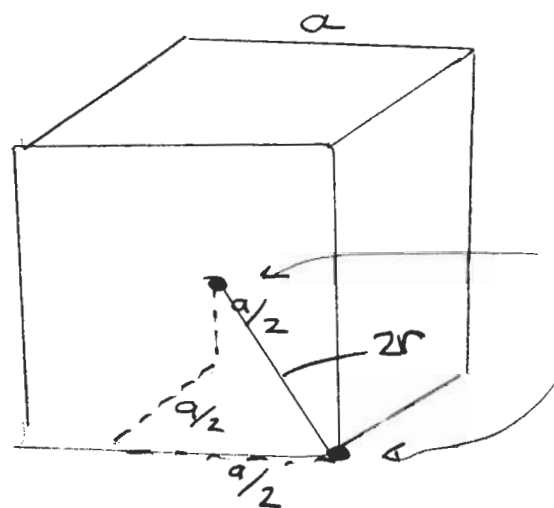
$$V_{\text{CUBE}} = a^3 = (2r)^3 = 8r^3$$

AT EACH CORNER,  $\frac{1}{8}$  OF AN ATOM IS CONTAINED  
WITHIN CUBE. SO TOTAL # ATOMS =  $8(\frac{1}{8}) = 1$ 

$$V_{\text{ATOMS}} = \frac{4}{3} \pi r^3 \quad (\text{VOLUME OF ONE SPHERE})$$

$$\text{PF} = \frac{V_{\text{ATOMS}}}{V_{\text{CUBE}}} = \frac{\frac{4}{3} \pi r^3}{8r^3} = \frac{\pi}{6} = 0.5236$$

$$= \boxed{52\%}$$

BCC:CENTERS OF  
2 TOUCHING  
ATOMS

$$\sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2} = 2r$$

$$\sqrt{\frac{3}{4} a^2} = 2r$$

$$\frac{3}{4} a^2 = 4r^2$$

$$a^2 = \frac{16}{3} r^2$$

$$a = \frac{4}{\sqrt{3}} r = \frac{4\sqrt{3}}{3} r = 2.3094 r$$

$$V_{\text{cube}} = a^3 = \left( \frac{4\sqrt{3}}{3} r \right)^3 = 12.3168 r^3$$

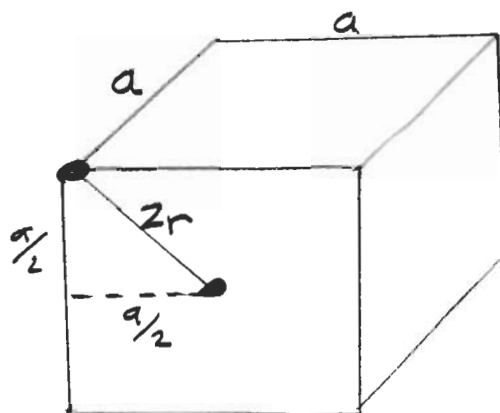
IN ADDITION TO  $\frac{1}{8}$  ATOM AT EACH CORNER,  
THERE IS A COMPLETE ATOM AT CENTER.

$\therefore$  2 ATOMS IN UNIT CELL

$$V_{\text{atoms}} = 2 \left( \frac{4}{3} \pi r^3 \right) = 8.3776 r^3$$

$$\text{PF} = \frac{V_{\text{atoms}}}{V_{\text{cube}}} = \frac{8.3776 r^3}{12.3168 r^3} = 0.6802$$
$$= \boxed{68\%}$$

FCC :



$$\sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2}$$
$$= 2r$$

$$\sqrt{\frac{1}{2} a^2} = 2r$$

$$\frac{1}{2} a^2 = 4r^2$$

$$a^2 = 8r^2$$

$$a = \sqrt{8}r = 2.8284r$$

$$V_{\text{cube}} = (\sqrt{8}r)^3 = 22.6274r^3$$

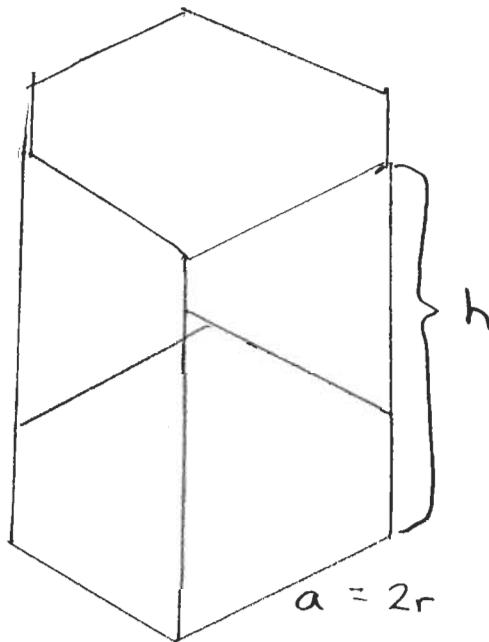
THERE IS  $\frac{1}{8}$  ATOM AT EVERY CORNER,  $\frac{1}{2}$  ATOM ON EACH OF THE 6 FACES.

$$\therefore \# \text{ ATOMS} = 8\left(\frac{1}{8}\right) + 6\left(\frac{1}{2}\right) = 4$$

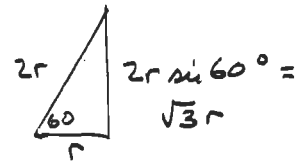
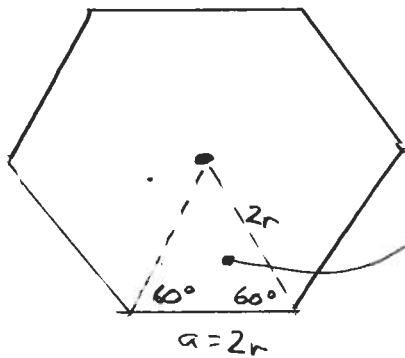
$$V_{\text{atoms}} = 4\left(\frac{4}{3}\pi r^3\right) = 16.7552r^3$$

$$PF = \frac{16.7552r^3}{22.6274r^3} = 0.7465 = \boxed{74\%}$$

HCP:



HEXAGON:



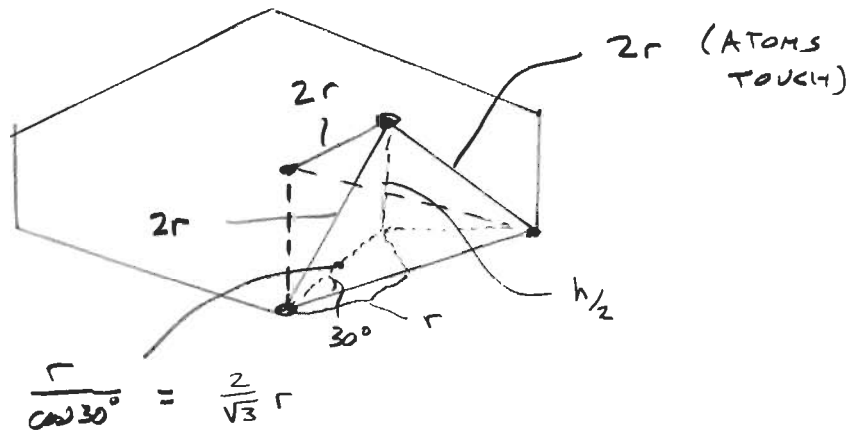
$$A = \frac{1}{2}bh$$

$$= \frac{1}{2}(2r)(\sqrt{3})r$$

$$= \sqrt{3}r^2$$

$$A_{\text{POLYGON}} = 6\sqrt{3}r^2$$

HEIGHT:



$$(2r)^2 = \left(\frac{2}{\sqrt{3}}r\right)^2 + \left(\frac{h}{2}\right)^2$$

$$\left(4 - \frac{4}{3}\right)r^2 = \frac{h^2}{4}$$

$$\frac{8}{3}r^2 = \frac{1}{4}h^2$$

$$\frac{32}{3}r^2 = h^2$$

$$3.2660r = h$$

$$V_{\text{CELL}} = Bh$$

$$= 6\sqrt{3}r^2(3.2660r)$$

$$= 33.9411r^3$$

# ATOMS (REFER TO PICTURE ON PAGE 17 OF STUDENT MODULE)

12 CORNERS - EACH  $\frac{1}{6}$  ATOM

TOP & BOTTOM - EACH  $\frac{1}{2}$  ATOM

MIDDLE ROW - 3 COMPLETE ATOMS

$$\# \text{ ATOMS} = 12\left(\frac{1}{6}\right) + 2\left(\frac{1}{2}\right) + 3 = 6$$

$$V_{\text{ATOMS}} = 6\left(\frac{4}{3}\pi r^3\right) = 25.1327 r^3$$

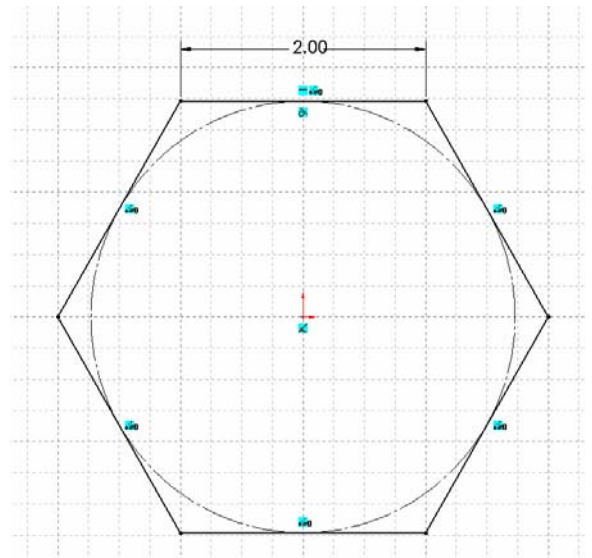
$$PF = \frac{25.1327 r^3}{33.9411 r^3} = 0.7405 = \boxed{74\%}$$

SEE FOLLOWING PAGES FOR  
CONSTRUCTION OF HCP  
UNIT CELL WITH SOLIDWORKS

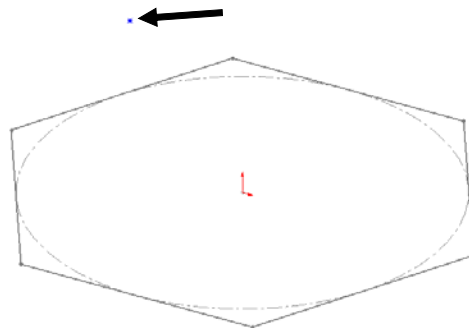
## Constructing the HCP unit cell with SolidWorks

Advanced students may want to construct the hexagonal close-packed structure. Here are the steps to do so.

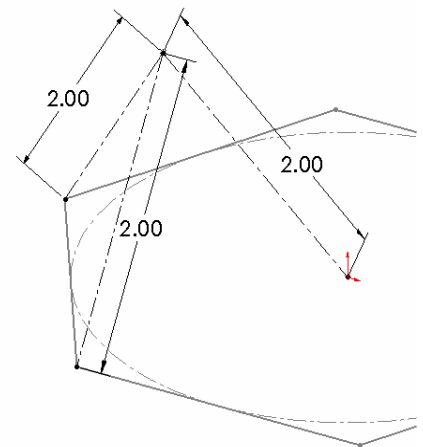
Open a new assembly. Create a new sketch in the Top plane, and create a hexagon (from Tools: Sketch Entities: Polygon). Make sure to center the hexagon at the origin. Add a 2-inch dimension to one side, and a horizontal relation to one side so that the sketch is fully defined. Close the sketch.



Open a 3D Sketch. Insert a point at a random location.

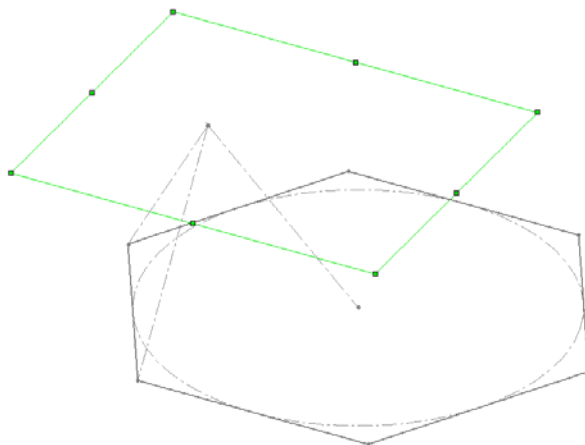


Add centerlines connecting the point to the origin (center of the hexagon) and two adjacent corners of the hexagon. Add 2-inch dimensions to each of the centerlines. This sets the position of one of the atoms on the middle row. This atom will touch three atoms on the lower row.

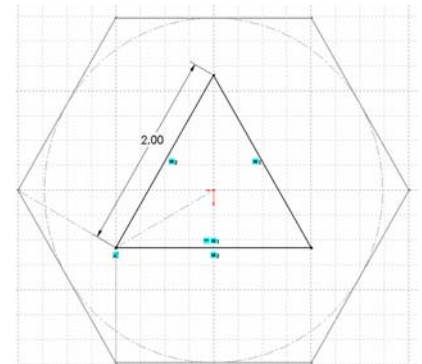


Close the sketch

Create a new plane. Select the Top Plane and the point just created to define the new plane (the new plane will contain the point and be parallel to the Top Plane).



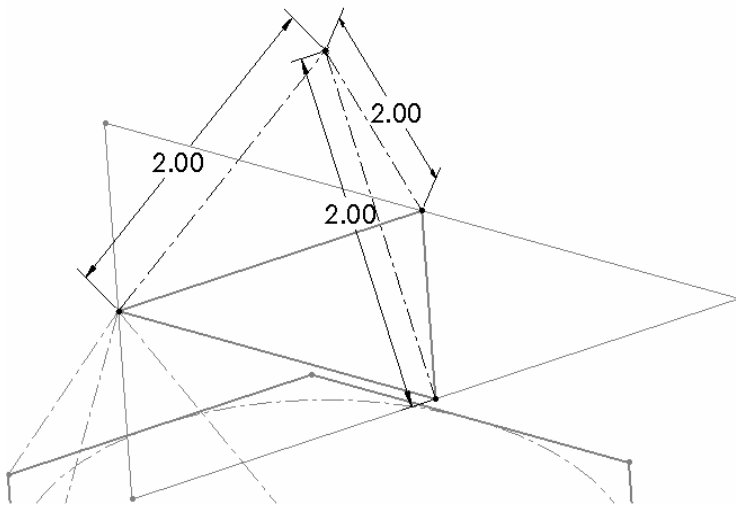
Open a sketch in the new plane. Add the three lines shown here. Use relations and a dimension to make the lines equal in length (2 inches). One line should be horizontal.



Add six more lines as shown, and use dimensions and/or relations so that they are all 2 inches in length.

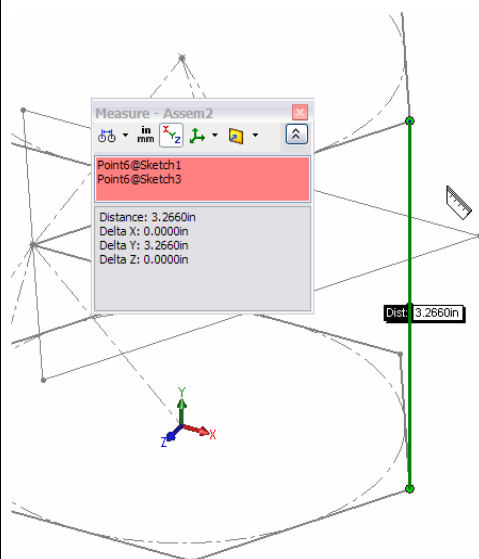
Close the sketch.

Open a new 3D sketch. Add a point, and add three centerlines connecting the point to corners of the center triangle of the previous sketch. Add 2-inch dimensions. The new point is the center of the top layer of atoms.

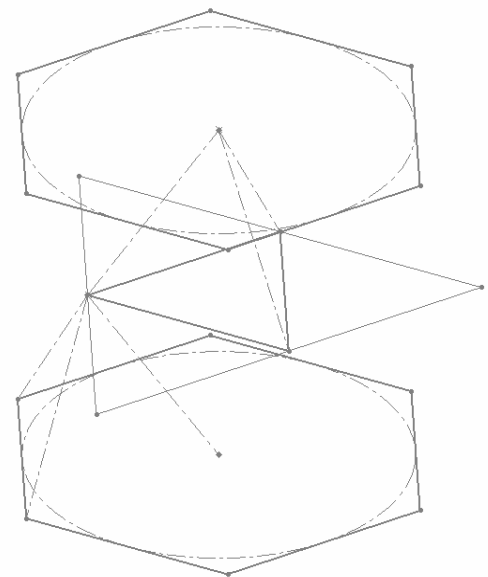
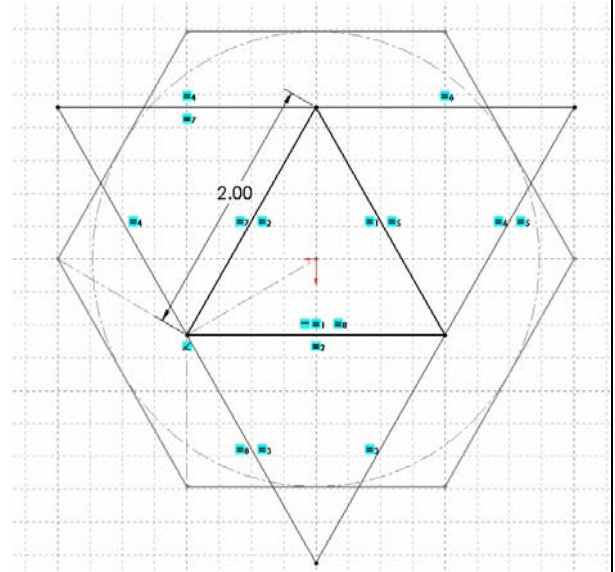


Close the sketch. Create a new plane through the point just created and parallel to the Top Plane.

Open a sketch in this plane, and create a hexagon directly above the first one.

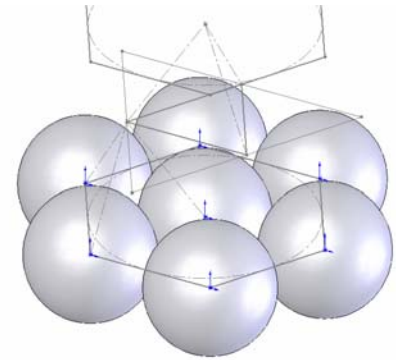
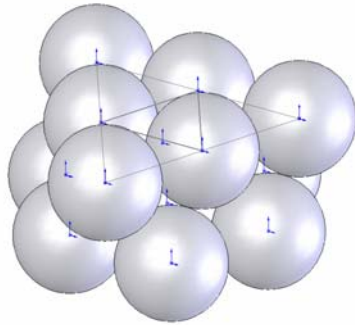


This completes the sketches needed to place the atoms in the assembly. Measure the overall height for use in calculating the packing factor.

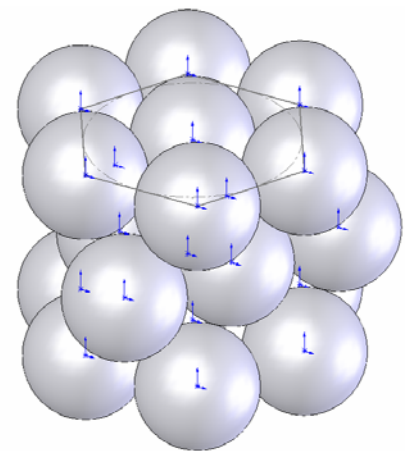


Add the atoms in layers:

Seven on the bottom:

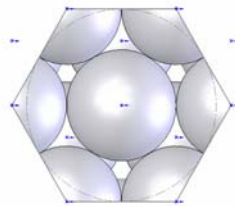


Six in the middle (note: hiding the sketches not needed is helpful):

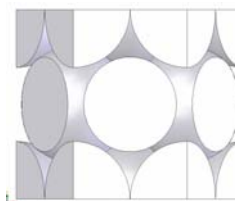
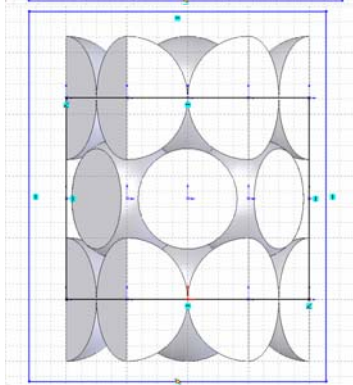
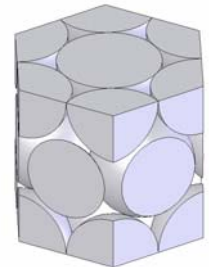


And seven on the top:

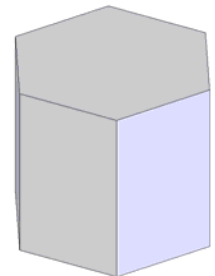
Cut away portions of atoms extending beyond the unit cell:



Check the mass properties (Volume = 25.1322 in<sup>3</sup>).



For the volume of the unit cell, create a separate part, using the height determined earlier, 3.2660 inches. (Volume = 33.9413 in<sup>3</sup>).



Packing factor =  $25.1322 / 33.9413 = 0.7405 = 74\%$ .