

Workshop: Packing of Hard Spheres

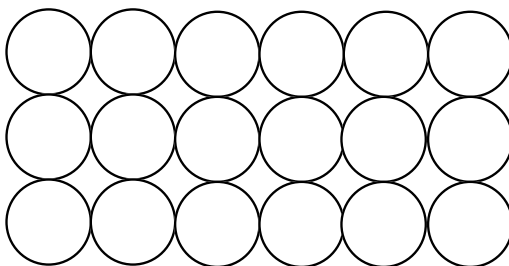
Form small groups of 2-3 people, so that you can easily see what's going on and use your hands. Each group will need: (a) a box, (b) about 40 plastic spheres, (c) about 10 blue glass marbles, (d) 90-100 colorless glass marbles, (e) a ruler.

Hints: It is easiest to get spheres to pack tightly if you tilt the box slightly toward one corner. You should consider having one person hold the box to keep everything together, while the other people stack the spheres... then alternate so everyone has a chance to play with the spheres.

Please be careful not to spill the spheres/marbles on the floor, or we will have a cleanup nightmare!

1. Use $2/3$ of the colorless glass marbles to make one cubic-packed layer.

Note the shape and size of the holes (gaps between the marbles). Try to stack marbles directly on top of each other to form a simple cubic lattice.



What does the difficulty tell you about the efficiency of this type of packing?

2. After making the first layer as shown above, stack the next layer of glass marbles into the holes of the first layer. (Place the second-layer marbles gently on the first layer, so you do not disturb the first-layer packing. If you try to make a second layer near the edge of your first layer, it will collapse.) **Are all the holes used?**

Draw the packing on the picture above. Continue with a third layer stacked into the holes of the second layer.

What kind of crystal packing is this: face-centered cubic or body-centered cubic?

What is the number of nearest neighbors for each marble?

How would you define a lattice point in this lattice?

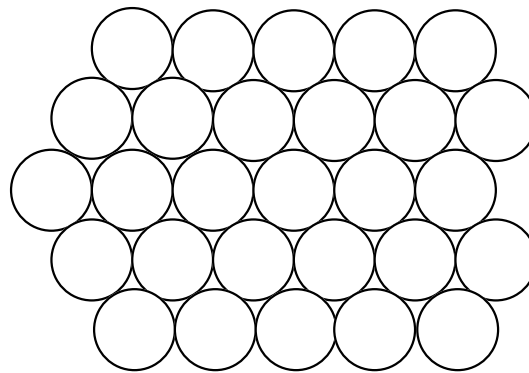
3. Finally, let's try alternating layers. Put in one cubic layer of plastic spheres, then fill the holes with glass marbles (very carefully, because the glass marbles are heavy and may fall through). Then, stack another layer of plastic spheres. Look at the plastic spheres only. **What is the packing structure of the plastic spheres now?**

What is the number of nearest neighbors, considering only the plastic spheres?

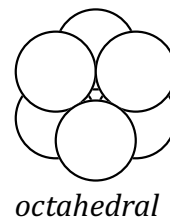
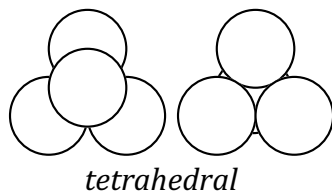
Compare to (1) and (2) above.

Hexagonal Packing:

4. Use 2/3 of the plastic spheres to make a hexagonal layer. (Hints for making a close-packed structure: (1) gently shake, (2) put a small piece of crumpled paper in the corner.) **Note the shape and size of the holes. Compare to (1).**



5. Place a second hexagonal layer of plastic spheres in the holes of the first layer. **Are all the holes used?**
6. Look for the octahedral and tetrahedral holes between the two layers.



These octahedral holes correspond to a position where there is a gap in *two* adjacent layers. **If it's really "close packed," why aren't all the holes capped by a sphere?**

7. Carefully place a third hexagonal layer of plastic spheres on your second layer (your third layer will only be 4-6 spheres). Your third layer can go on top of either the tetrahedral holes or the octahedral holes created by the first two layers. If you stack on the tetrahedral holes, the octahedral holes will line up to form infinite columns of empty space in your structure. This is *hexagonal close packing* (hcp), and your 1st and 3rd layers are directly on top of one another (ABAB...)

What is the number of nearest neighbors to each sphere?

How would you define the lattice points of this lattice?

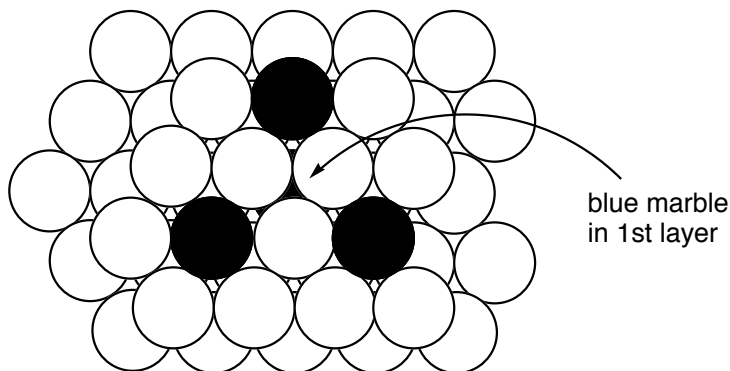
8. If you stack the third layer on the octahedral holes, you have created *cubic close packing* (ccp), and all three layers are shifted with respect to one another (ABCABC...)

What is the number of nearest neighbors to each sphere?

9. Finally, we need to see that ccp is the same as face-centered cubic (fcc). To create the cubic unit cell, you will create 4 close-packed layers. You will use the blue and clear glass marbles for this exercise, and the blue marbles will define the points of the cube.

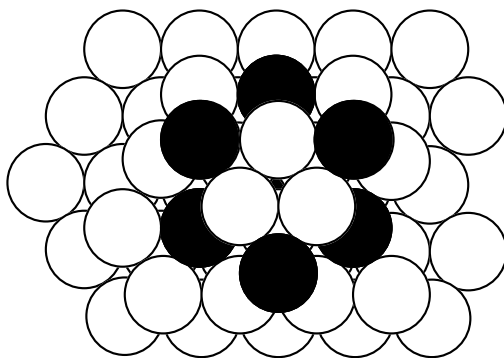
a) Make a large close-packed layer with about 2/3 of your colorless glass marbles. Include a single blue marble in the center of a well-packed area.

b) Add a second layer using colorless glass marbles, except include three blue marbles as shown (note their position with respect to the blue marble in the first layer):



The vertical line down through the first-layer blue marble will be the C_3 axis of the cube: note the three-fold symmetry in your blue pattern.

c) Add a third layer of three clear and three blue marbles as shown in the picture below.
Is this hcp or ccp?



d) Finally, place one last blue marble (a fourth layer) on the center of the pattern. The eight blue marbles are the corners of a cube sitting on one corner! This cube is the fcc unit cell. Can you see the *body diagonal* of the cube (which is perpendicular to the base of the box)? Look at the locations of the clear marbles within this unit cell.

Are any marbles in the center of the cube?

Do all six faces of the cube contain a clear marble?

How many of each color marble are in the unit cell that corresponds to the cube?

e) This shows that ccp (cubic close packing) is the same as fcc (face-centered cubic). There are interesting patterns along tilted planes in an fcc crystal: square, hexagonal (other than the horizontal one), etc.

Find these in your remaining time.