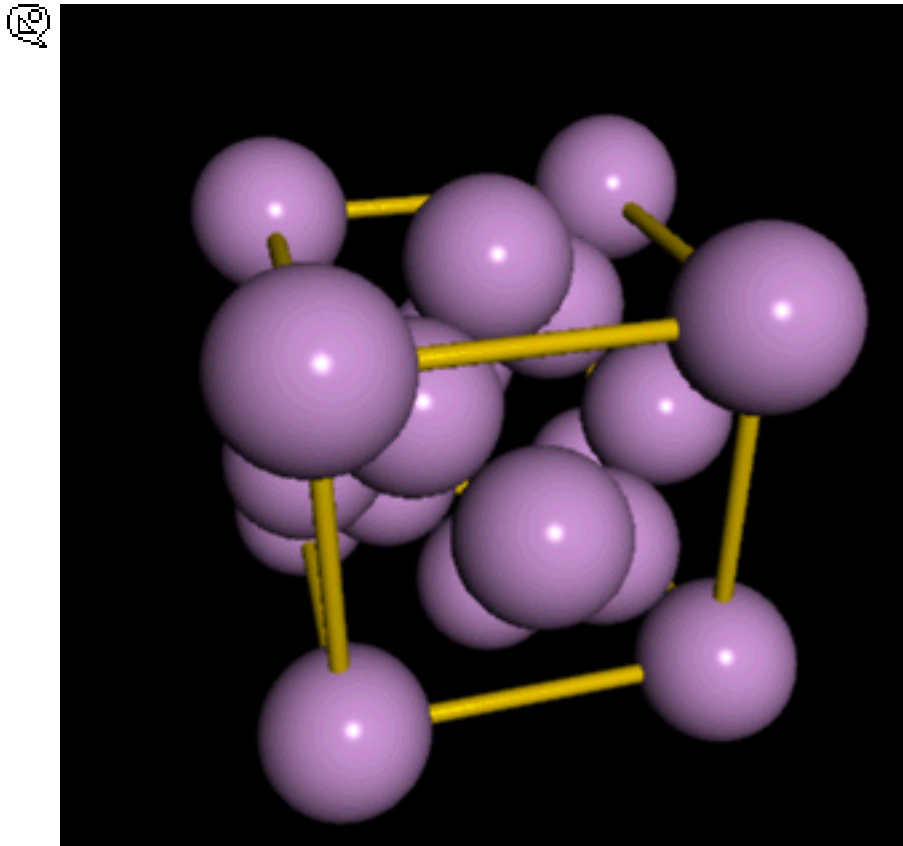


Example 3-4 (Askeland Example 03-15)
Packing Factor in Diamond Cubic Structure.

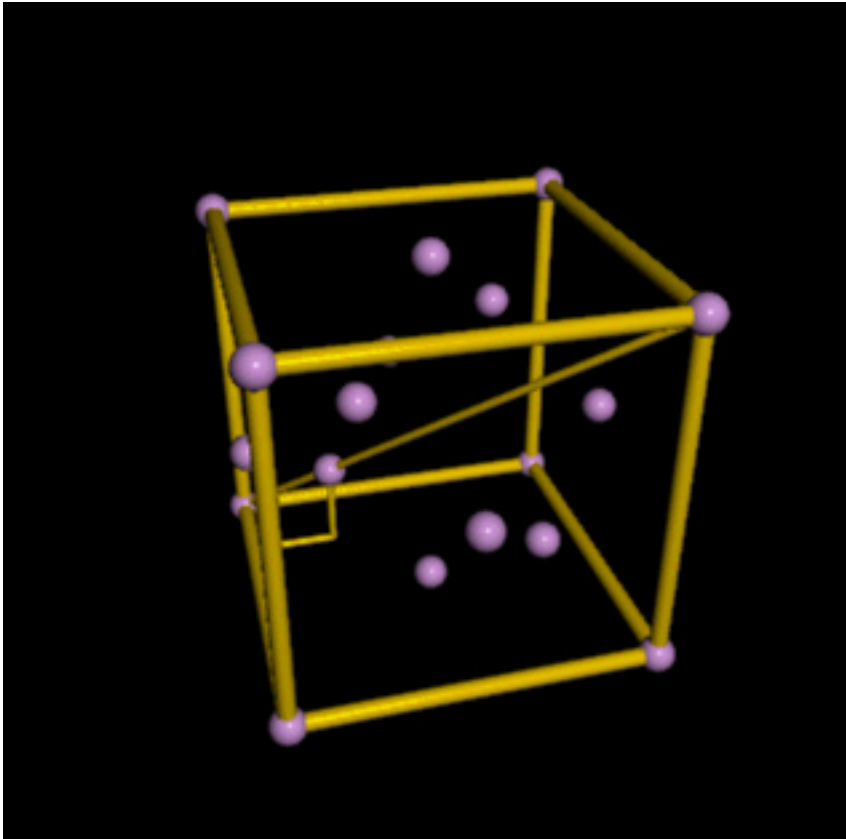
Determine the packing factor in DC silicon.

This is often one of the more difficult unit cells for students to calculate the packing factor. The geometry that relates the size of the unit cell to the size of the atoms is more difficult to visualize because the atoms do not line up in a continuous touching line in the body diagonal direction.

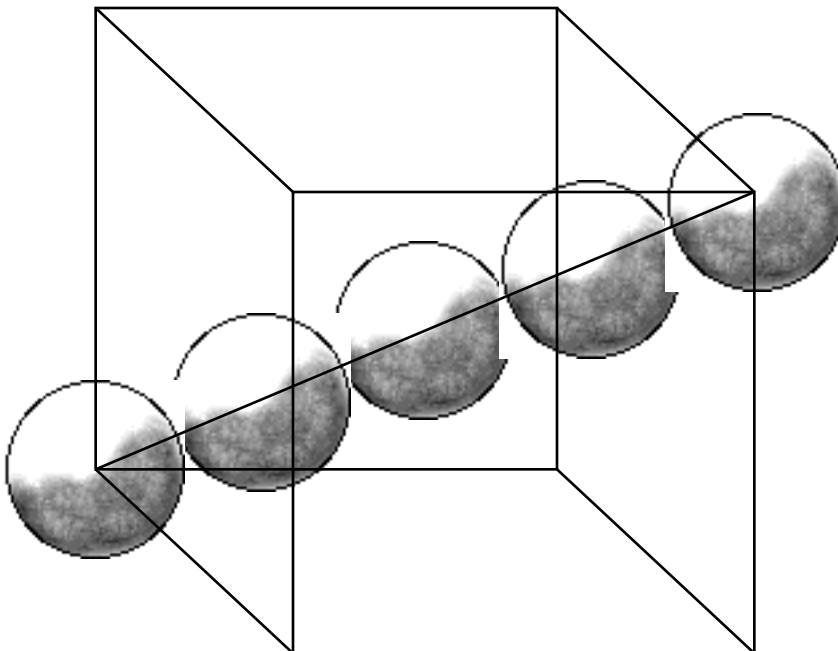
The image below shows the diamond-cubic unit cell, with space filling atoms. This unit cell has a face-centered cubic lattice, with two atoms as the basis. If you place a pair of touching atoms, one at coordinates $(0, 0, 0)$ and the other at $(1/4, 1/4, 1/4)$ at each of the lattice points it generates the diamond cubic structure. Each of these atoms touches four others, which are arranged around the atom in a tetrahedral configuration. Since the silicon atoms are covalently bonded to each other, the tetrahedral arrangement allows the bonds (where the electrons are localized) to be maximally separated from each other. To see the tetrahedral arrangement of atoms in the image below, consider one of the atoms at the internal sites (with coordinates $1/4, 1/4, 1/4$). This atom touches four others - the one at the nearest corner and three atoms in the center of the nearest faces.



It is somewhat easier to see the atom relationships if we shrink down the atoms, and add a few construction lines. In the sketch below, only the atom centers are shown. Also, in addition to the edges of the cubic unit cell, there is a line shown along the body diagonal of the cell that passes through one of the atoms at the tetrahedral site inside the cell. This atom is at coordinates of $(1/4, 1/4, 1/4)$, as shown by the construction lines parallel to the edges that show its coordinates.



The textbook suggests one way to relate the atom dimension to the unit cell. It notes that IF additional atoms were inserted along the diagonal, they would just fit. Then the diagonal line through the cubic unit cell would have a length exactly equal to 4 times the atom diameter.



This line has a length equal to 8 times the radius of the atom, but it is also equal to the body diagonal of the cube, or $\sqrt{3}$ times a (the edge of the cube). Hence

$8r = \sqrt{3} a$

$$\triangle a = 4.62 r$$

☰ There is actually an easier way to reach the same conclusion. Refer back to the image showing the atoms reduced in size, with the diagonal line. Notice that the line passes through the atom at the 1/4, 1/4, 1/4 point. The distance from this point to the corner is just twice the radius of the atoms. But in terms of the coordinates, the Pythagorean theorem tells us that the length of the line segment is

$$\square 2r = \sqrt{\left(\frac{1}{4}a\right)^2 + \left(\frac{1}{4}a\right)^2 + \left(\frac{1}{4}a\right)^2}$$

$$\triangle 2r = \sqrt{3(0.25a)^2}$$

☰ Solving this for a give two possible solutions, but only the positive one has physical meaning

$\triangle a = 4\sqrt{\frac{1}{3}(2r)^2}$	$\triangle a = -4\sqrt{\frac{1}{3}(2r)^2}$
---	--

☰ This simplifies to the same answer as the other method (as of course it must). The reason for showing two different approaches to solving for the relationship between a and r is to help you understand the geometry of the unit cell.

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

$$\triangle a = 4.62 r$$

☰ Now we can proceed to calculate the packing factor. This is defined as the volume occupied by the atoms divided by the volume of the unit cell.

$$\blacksquare \text{PF} = \frac{N \frac{4}{3} r^3}{a^3}$$

☰ N is the number of atoms per unit cell. We can determine this in three different ways, all of which give the same result. You may either select the method that you visualize best, or by understanding them all and how they relate, further develop your familiarity with the idea of a unit cell.


A. We can count the fractions of atoms within the bounds of the unit cell, referring to the first image shown above. This would give
 8 corner atoms * 1/8 +
 6 face-centered atoms * 1/2 +
 4 internal atoms
 = 8 total atoms per unit cell.

B. We can count those atoms whose coordinates (x,y,z) have values of x, y and z that are greater than or equal to zero but strictly less than one. A complete list of such atoms is (0,0,0) - the corner atom at the origin. Other corner atoms have at least one coordinate of 1 and are therefore not counted.
 (1/2, 1/2, 0); (1/2, 0, 1/2); (0, 1/2, 1/2) - three face atoms. Other face atoms have at least one coordinate of 1 and are therefore not counted.
 (1/4, 1/4, 1/4); (3/4, 3/4, 1/4); (1/4, 3/4, 3/4); (3/4, 1/4, 3/4) - the four internal atoms at tetrahedral sites.
 This gives a total of eight atoms.

C. We can use the fact that the unit cell has an FCC lattice and a basis of two atoms per lattice point. The FCC lattice has four points per unit cell, so two times four equals 8.

Each of these methods gives us N=8 as the number of atoms per unit cell.


$N = 8$

 For convenience, the relationship between a and r , and the packing factor equation are reproduced below. If we drag the value for N and the equation for a into the expression, we can solve for the packing factor.

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


$PF = \frac{N \frac{4}{3} \pi r^3}{a^3}$

$PF = \frac{32}{3} \pi r^3 \frac{1}{(4.62 r)^3}$

 In order to solve this expression, we first tell Theorist to expand the expression, which expands the r^3 in the denominator so that it cancels the r^3 in the numerator, and then calculate the numeric result.

$PF = 0.108 \pi$

$PF = 0.34$

 The final answer is a packing factor of 0.34, which is much lower than metallic unit cells (BCC=0.68, FCC=0.74), or most ionic structures. This is because of the strong covalent bonding in diamond cubic materials.