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What is Atomic Packing Factor (and How to Calculate it for SC, BCC, FCC, and HCP)?



Atomic Packing Factor (APF) tells you what percent of an object is made of atoms vs empty space. You can think of this as a **volume density**, or as an indication of how tightly-packed the atoms are.

For quick reference, I have created a table below of **atomic packing factor** (APF) values for **common crystal structures**. Later in the article, I explain step-by-step how to calculate them.

Crystal Structure	Atomic Packing Factor
Simple Cubic (SC)	52%
Body-Centered Cubic (BCC)	68%
Face-Centered Cubic (FCC)	74%
Hexagonal Close-Packed (HCP)	74%

Atomic packing factor (APF) of common crystal structures.

Calculating the **atomic packing factor** for a crystal is simple: for some repeating volume, calculate the volume of the atoms inside and divide by the total volume.

$$APF = \frac{\text{volume taken by atoms}}{\text{total volume}}$$

Usually, this “repeating volume” is just the volume of the unit cell. The unit cell is defined as the simplest repeating unit in a crystal.

Assuming all atoms have the same size, and are arranged in a repeating crystal lattice,

$$APF = \frac{N_{atoms} V_{atom}}{V_{unit\ cell}}$$

where N means number and V means volume.

► **For a more complicated description of having multiple kinds of atoms, click here to expand.**

Additionally, atomic packing factor uses the hard sphere model. That means each atom has the volume of a sphere. Assuming the atoms are hard spheres with radius r in a cubic unit cell with lattice parameter a ,

$$APF = \frac{\frac{4}{3}\pi r^3 \cdot N_{atoms}}{a^3}$$

This might be a little hard to conceptualize, so let's start by dropping into 1- and 2- dimensions.

Outline

- 1-Dimensional Packing Factor: Linear Density
- 2-Dimensional Packing Factor: Planar Density
- Simple Cubic (SC) Lattice Length and APF
- Body-Centered Cubic (BCC) Lattice Length and APF
- Face-Centered Cubic (FCC) Lattice Length and APF
- Hexagonal Close-Packed (HCP) Structure and APF
- Final Thoughts

1-Dimensional Packing Factor: Linear Density

Since we're in 1D, formulas with volume don't apply. Don't worry! If you understand the concept, you won't need a formula at all.

Remember, we want to find the space taken by atoms compared to the total space. Since we're in 1-dimension, "space" means "length." We can say that 1-dimensional packing is a **linear density** or line density.

For any particular direction, you need to draw a line and determine what percent of the line is covered by a circle.

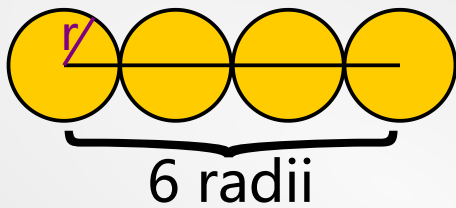
Of course, you can't just draw any random line. The line needs to be along the crystal "cell."

► **If you're not sure how to do this in 1-dimension, click here to expand.**

As long as the line you draw is a valid representation of the overall crystal symmetry, any line will work!

Simply take the length of the line covered by circles, and divide by the total length of the line.

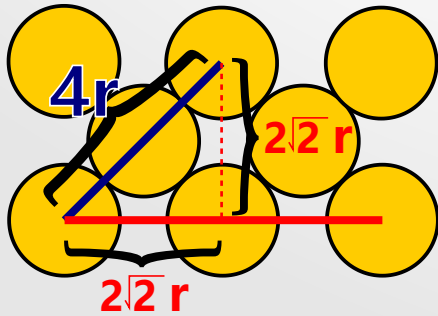
1-Dimensional Packing Factor: Linear Density



Length of circles on the line: $6r$
 Length of line: $6r$

$$\text{APF} = 1 \text{ or } 100\%$$

100% of the line is occupied by circle, so the packing is 100%



Blue Line has APF = 1

What about the Red Line?

Length of circles on the red line: $4r$

Length of red line: $2 \times 2\sqrt{2}r$

$$\frac{4r}{4\sqrt{2}r}$$

$$\text{APF} = \frac{\sqrt{2}}{2}$$

or 74.07%

So 74.07% of the red line is occupied by a circle

The maximum packing factor is 1, which means 100% of the line is occupied by a circle.

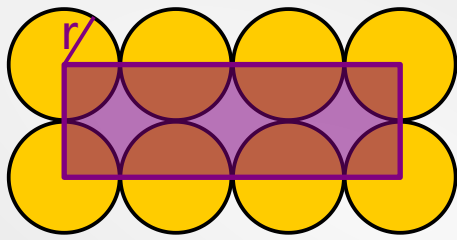
If you had a packing factor larger than one, it would mean that somehow multiple circles overlapped on the same section of the line.

2-Dimensional Packing Factor: Planar Density

In 2 dimensions, space is *area*, rather than a line or a volume. Determining the packing factor works exactly the same way, however. We call this the **planar density** or area density.

Simply find a crystallographically repeating area (the unit cell will always work) and divide that area by the area covered by the circles.

2-Dimensional Packing Factor: Planar Density



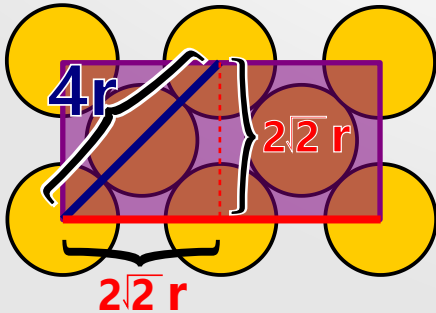
Area of circles in the box: $4 \times \frac{1}{4} \pi r^2 + 4 \times \frac{1}{2} \pi r^2$

Area of box: $2r \times 6r$

$$APF = \frac{3\pi r^2}{12r^2}$$

or 78.54%

So 78.54% of the box is occupied by circles



Area of circles in the box: $4 \times \frac{1}{4} \pi r^2 + 2 \times \frac{1}{2} \pi r^2 + 2\pi r^2$

Area of box: $2\sqrt{2}r \times 4r$

$$APF = \frac{4\pi r^2}{16r^2}$$

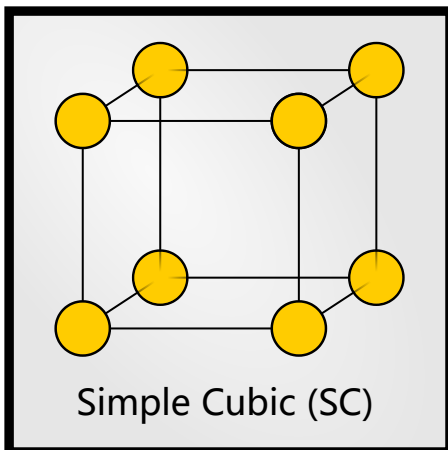
or 78.54%

Both 2-Dimensional crystals have equal packing!

Look at that! These two arrangements have the same packing. Any idea why that is ... ?

Now, let's move into 3 dimensions and take a look at how to calculate APF for the 4 common unit cells.

Simple Cubic (SC) Lattice Length and APF



As before, we want to know how much of the crystal space is occupied by atoms vs empty space. We have entered 3-dimensions (the real world), so space is **volume**. To perform this calculation, we need to know the volume of a cube and the volume of a sphere.

Volume of a cube: $V_{cube} = a^3$, where a is the length of a side.

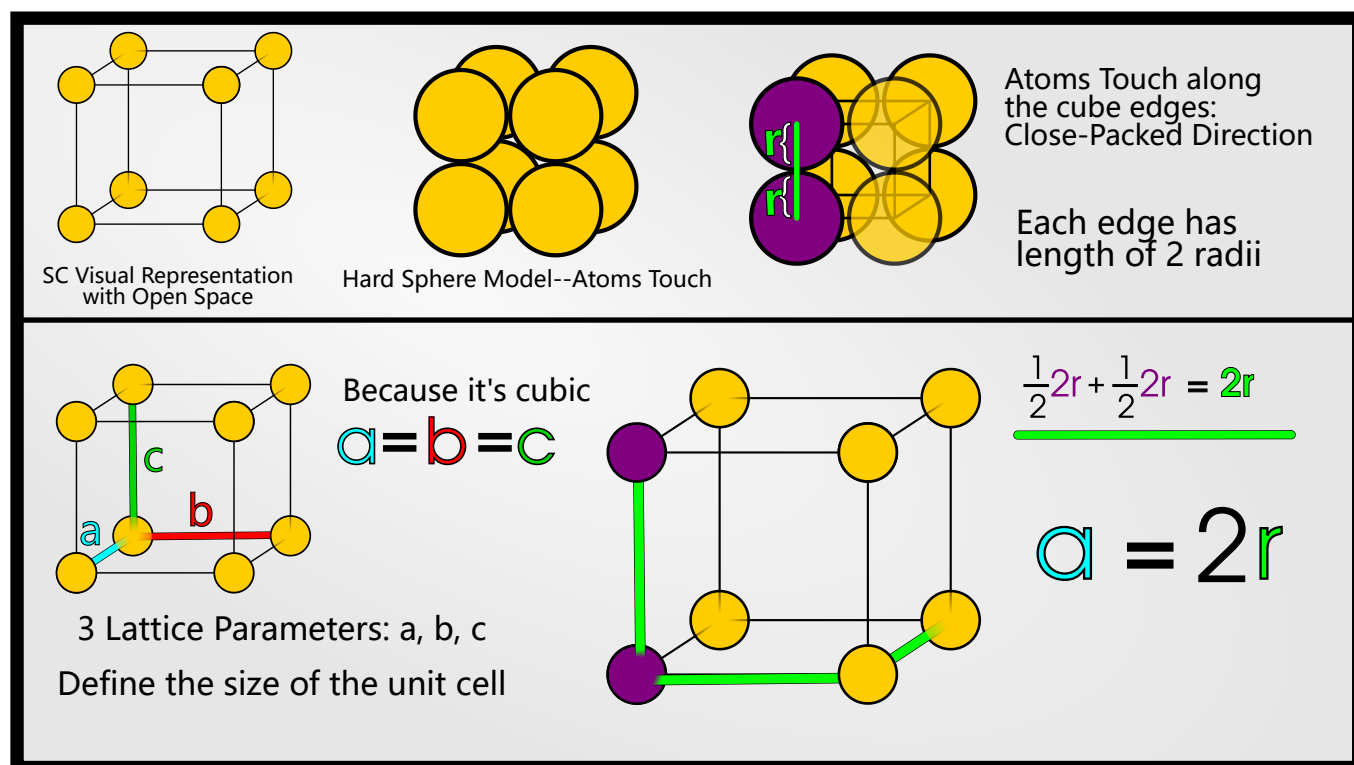
Volume of a sphere: $V_{sphere} = \frac{4}{3}\pi r^3$, where r is the radius

of the sphere.

Now, we have 2 variables: r (radius of atom) and a (side length of cube).

It turns out that r and a can be written in terms of each other.

A simple cubic (SC) unit cell is a cube with an atom on each corner of the cube. The size of the cube will be determined by the size of the atoms!



As you can see, for the simple cubic cell, the lattice parameter is just twice the radius. Now, in terms of the radius, we can say that the **volume of the cube** is:

$$V = (2r)^3 = 8r^3$$

Each atom is a **sphere**, so the **volume per atom** is:

$$V_{\text{sphere}} = \frac{4}{3}\pi r^3$$

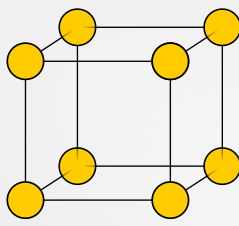
where r is the radius of the sphere.

But, how many atoms do we have per unit cell? At first glance, it looks like there are 8 atoms: one on each corner of the cell.

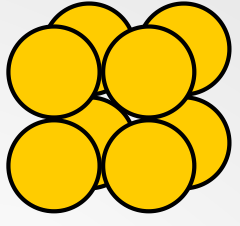
However, you need to consider that when you stack unit cells to make the full crystal, each corner is shared with 8 cells. So each of the 8 atoms contributes $\frac{1}{8}$ of its total volume. In total, there is 1 full atom per unit cell.

Now if we divide the volume of an atom by the volume of the unit cell, the **atomic packing factor for a simple cubic crystal** is:

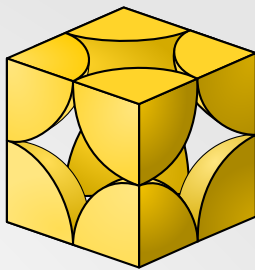
$$APF_{SC} = \frac{\frac{8}{8} \cdot \frac{4}{3}\pi r^3}{(2r)^3} = \frac{\pi}{6} \approx 52\%$$



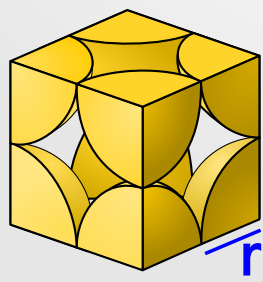
Simple Cubic
Open Visualization



Simple Cubic
Hard Sphere Model



Cut-out showing
the amount of
each atom strictly
inside the unit cell



2r
r

$$APF = \frac{\text{Volume of atoms}}{\text{Volume of unit cell}}$$

Volume of atoms = $\frac{8}{8} \cdot \frac{4}{3}\pi r^3$

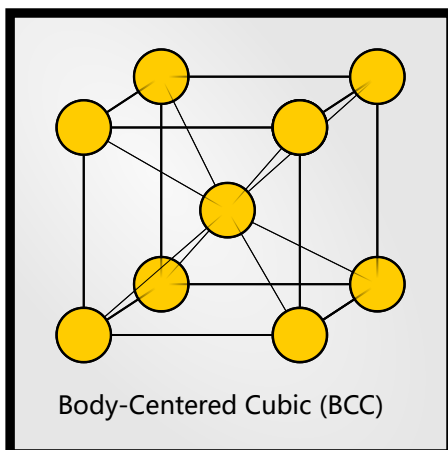
Volume of cube = $8r^3$

8 atoms on each corner,
but each atom only has
1/8 of its volume inside
the unit cell

For Simple Cubic

$$APF = \frac{\pi}{6} = 52\%$$

Body-Centered Cubic (BCC) Lattice Length and APF



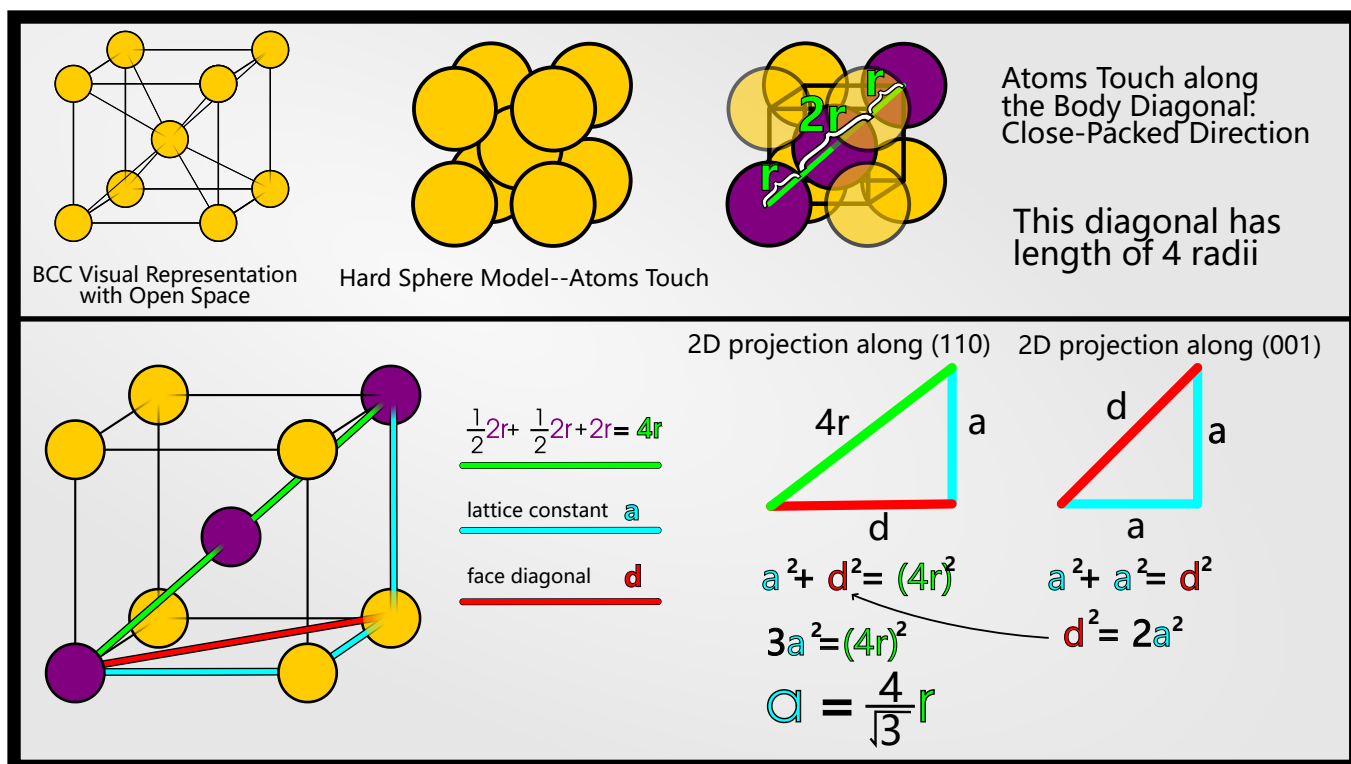
To calculate the atomic packing factor, what do we need first? The volume of the atoms, and the volume of the unit cell.

For some radius of the atoms, we can calculate their volume using

$$V_{sphere} = \frac{4}{3}\pi r^3$$

The volume of the cube is a^3 in terms of the lattice constant a , so let's write a in terms of r .

In a BCC crystal, the **body diagonal** is the close-packed direction. I hope this is clear in the image below.



Since the body diagonal is the close-packed direction, the atoms touch each other. That means the body diagonal will be a multiple of the atomic radius. In this case, the body diagonal is $4r$.

Now, it's time to use the pythagorean theorem (you could also use 3D vector math, but if you don't know what that is, the trigonometry is not so complicated).

First, make a triangle with the body diagonal as the hypotenuse. This is the green line in the image above. One of your triangle legs will be the cube's side, a . The other leg will be the face diagonal. You can use any variable you like for this length; I will choose d .

Using the pythagorean theorem, $a^2 + d^2 = (4r)^2$.

Now, let's find d . We can make another triangle from a different 3D view; this time our triangle has d on the hypotenuse and a for both legs.

Again using the pythagorean theorem, we see $a^2 + a^2 = d^2$, or $d^2 = 2a^2$.

Now we can plug d^2 into our first pythagorean theorem.

$$a^2 + 2a^2 = (4r)^2$$

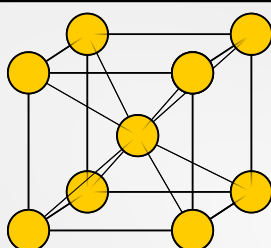
So,

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

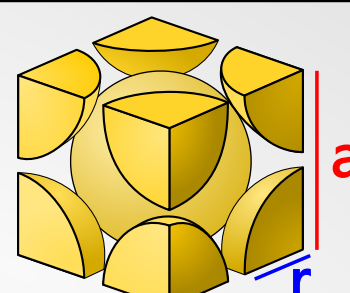
Now that we can write the volume of the cube in terms of the atomic radius, the rest is easy!

We only need to figure out how many atoms are in each unit cell. As in the simple cubic example, there are 8 corner atoms. Each corner atom contributes $\frac{1}{8}$ of its volume to the unit cell, so that's equal to 1 whole atom.

Additionally, there is an atom in the middle of the cell. Since that entire atom is inside the cell, it fully contributes its volume.



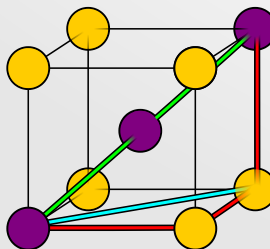
Body-Centered Cubic
Open Visualization



8 atoms on each corner,
with $\frac{1}{8}$ of its volume
inside the unit cell

+ 1 full atom inside

= 2 atoms per unit cell



$a^2 + d^2 = (4r)^2$

$d^2 = 2a^2$

APF = $\frac{\text{Volume of atoms}}{\text{Volume of unit cell}}$

Volume of atoms = $2 \cdot \frac{4}{3}\pi r^3$

Volume of cube = $\left(\frac{4}{\sqrt{3}}r\right)^3$

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

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

For BCC

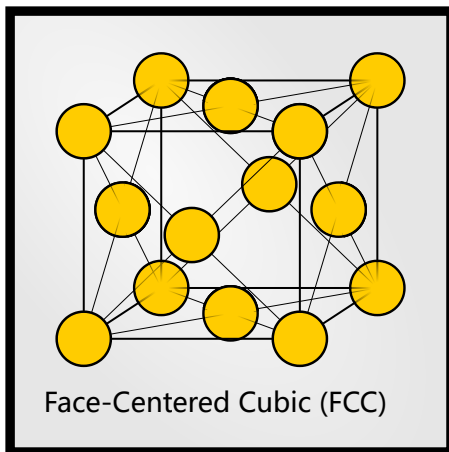
APF = $\frac{\sqrt{3}\pi}{8} = 68\%$

In total, there are **2 atoms** in the BCC unit cell. If we divide the volume of 2 atoms by the volume of the unit cell ($= a^3$), we find that the **atomic packing factor for a body-centered cubic crystal** is:

$$APF_{BCC} = \frac{\left(\frac{8}{8} + 1\right) \frac{4}{3}\pi r^3}{\left(\frac{4}{\sqrt{3}}r\right)^3} = \frac{\sqrt{3}\pi}{8} \approx 68\%$$

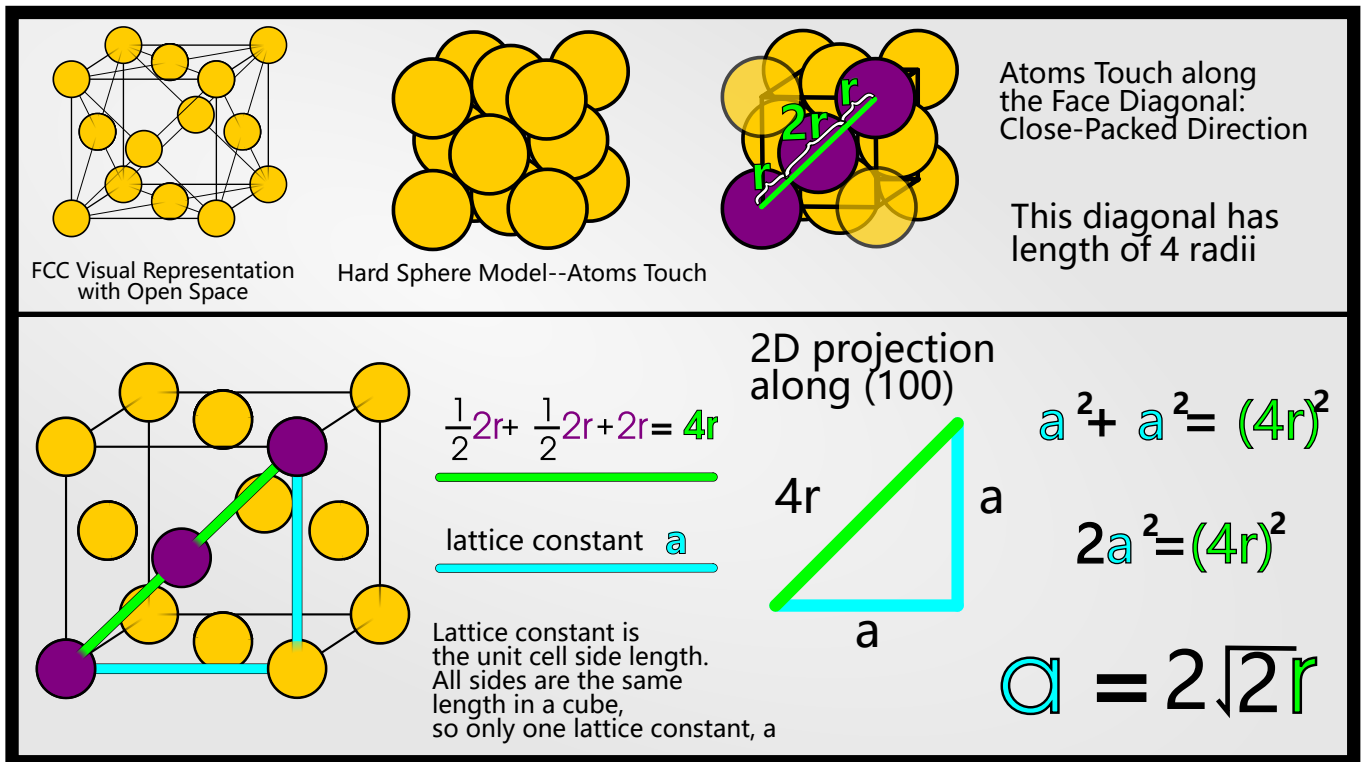
Face-Centered Cubic (FCC) Lattice Length and APF

This should be familiar by now. Volume of the atoms divided by volume of the unit cell. Let's get the unit cell in terms of the atomic radius!



In an FCC crystal, any **face diagonal** is the close-packed direction. I hope you can see this in the image below.

The face diagonal, therefore, has a length of $4r$. We can get the lattice constant in terms of r with a simple application of the pythagorean theorem.



Draw a triangle with the face diagonal (length $=4r$) as the hypotenuse. Both legs will be a .

$$a^2 + a^2 = (4r)^2$$

$$\text{So } a = 2\sqrt{2}r$$

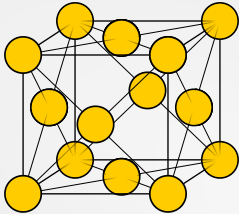
a^3 will be the volume of the unit cell, so let's figure out how many atoms are in the unit cell.

As we've seen several times already, there will be 8 atoms on each corner, each contributing $\frac{1}{8}$ of its total volume to the unit cell.

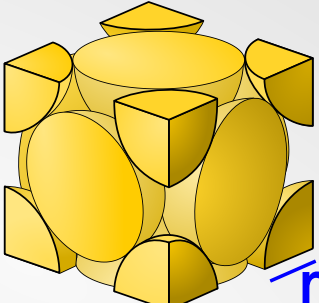
Additionally, there are 6 faces, with half an atom on each face (since faces are shared between two cells, an atom on the face would contribute $\frac{1}{2}$ of its volume to each cell).

In total, there are 4 atoms in the FCC unit cell. Dividing the volume of 4 atoms by the volume of the cube gives us the **atomic packing factor for a face-centered cubic crystal**:

$$APF_{FCC} = \frac{\left(\frac{8}{8} + \frac{6}{2}\right) \frac{4}{3}\pi r^3}{(2\sqrt{2}r)^3} = \frac{\pi}{3\sqrt{2}} \approx 74\%$$



Face-Centered Cubic
Open Visualization

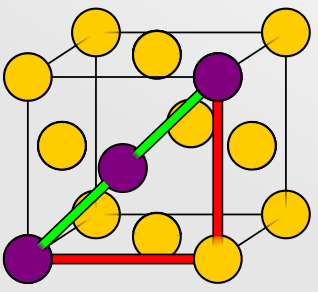


a
 r

8 atoms on each corner,
with $\frac{1}{8}$ of its volume
inside the unit cell (1)

+ 6 atoms on each face
with $\frac{1}{2}$ of its volume
inside the unit cell (3)

= 4 atoms per unit cell



$4r$
 a

$a^3 = 16\sqrt{2}r^3$
 $2a^2 = (4r)^2$
 $a = 2\sqrt{2}r$

$APF = \frac{\text{Volume of atoms}}{\text{Volume of unit cell}}$

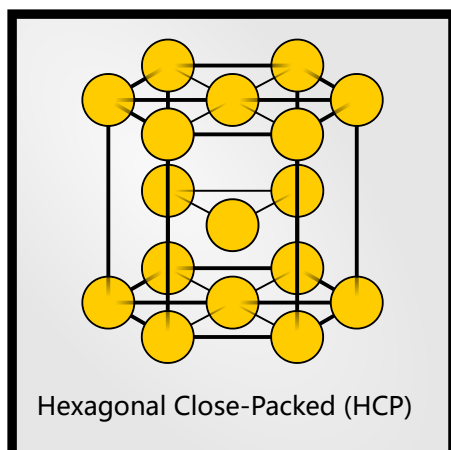
Volume of atoms = $4 \cdot \frac{4}{3}\pi r^3$

Volume of cube = $(2\sqrt{2}r)^3$

For FCC

$APF = \frac{\pi}{3\sqrt{2}} = 74\%$

Hexagonal Close-Packed (HCP) Structure and APF

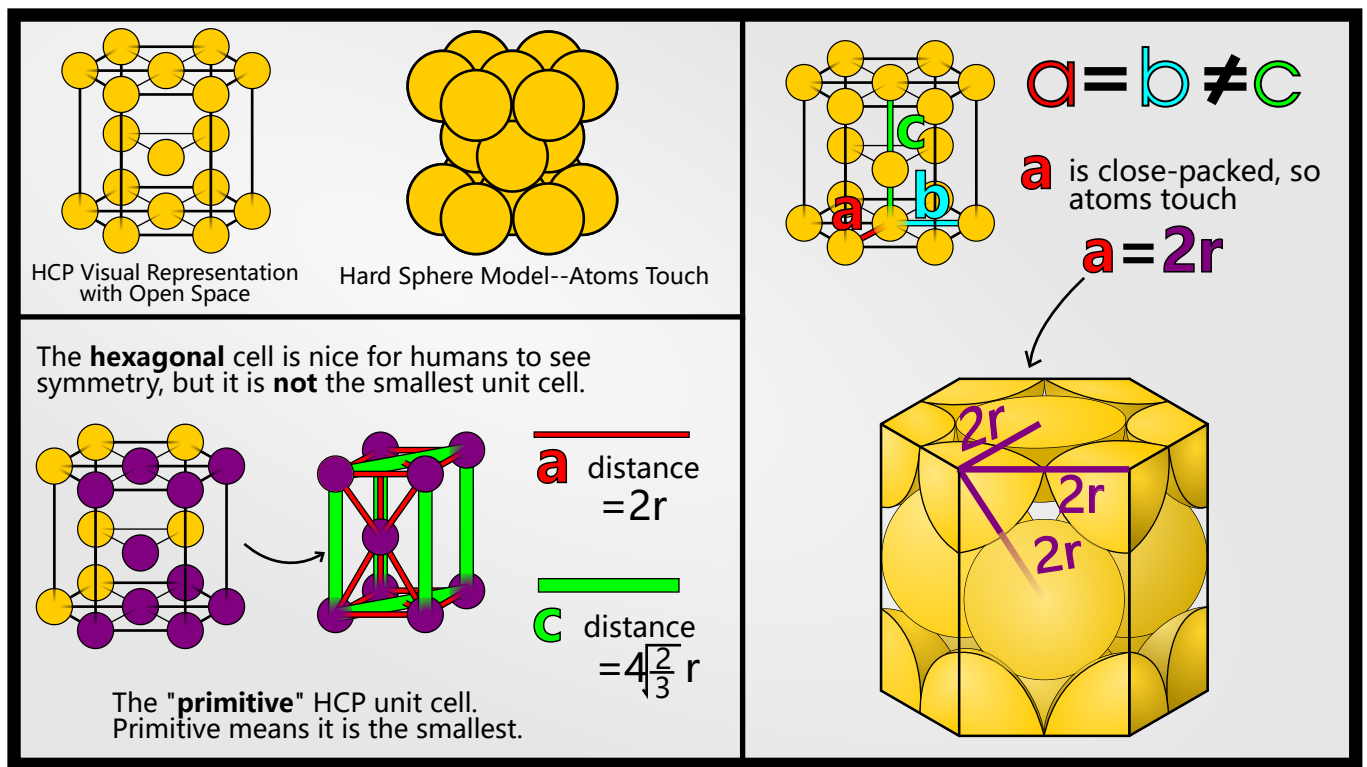


Now things become tricky.

The HCP crystal structure is *not* cubic. Luckily, it's still relatively easy to visualize. It's the natural way for humans to pack spheres.

Imagine you had to pack spheres into a box. You'd probably start by making a close-packed plane on the bottom of the box. Then, you'd start the next plane by placing a sphere at one off the low points—in between 3 spheres from the bottom plane. Again, the 2nd plane can be arranged as close-packed. The 3rd plane would look exactly like the 1st plane, the 4th plane would look exactly like the 2nd plane, and so on.

This is the hexagonal close-packed lattice!



We call this unit cell “hexagonal close-packed” because it looks like hexagonal planes. In almost all cases, we use the full HCP cell.

However, it’s actually possible to define a smaller unit cell from the same atomic arrangement. This is a **rhombohedral** cell. Since this is the smallest unit cell possible, we call this the HCP **primitive unit cell**.

Let’s look at the primitive unit cell, because it’s simpler so it’s easy to see the lattice parameters. Unlike a cube, there are actually **2** independant lattice parameters.

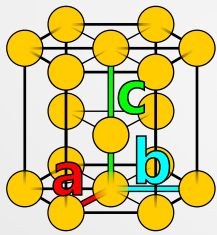
Lattice parameter $a = b$ is the length between 2 touching atoms (so, twice the radius).

Lattice parameter c is the height of the unit cell.

By taking advantage of some trigonometry, it turns out that in an ideal HCP cell, there is a definite ratio of c/a .

The Hexagonal Close-Packed c/a ratio

Hexagonal Close-Packed c/a ratio



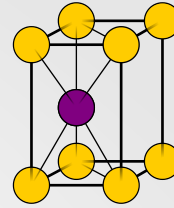
$$a = b \neq c$$

a is close-packed, so atoms touch

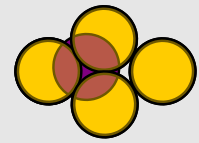
$$a = 2r$$

$$c = ?$$

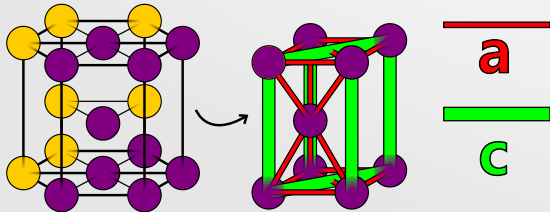
This central atom is touching 6 other atoms in the primitive cell



Top view



What is **c**, the height of the prism?



The **primitive cell** will make this simple

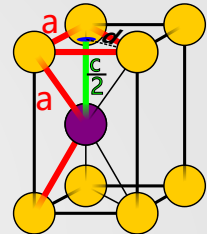
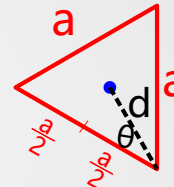
$$\theta = 30^\circ$$

$$\cos(\theta) = \frac{\frac{a}{2}}{d}$$

$$d = \frac{a}{\sqrt{3}}$$

$$\left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 = a^2$$

$$c = \sqrt{\frac{8}{3}} a$$



Lattice Parameter **c**

$$c = \sqrt{\frac{8}{3}} a = 4\sqrt{\frac{2}{3}} r$$

If you look at the central atom in the primitive cell, you can see that it has a distance a between the atoms in the plane above and in the plane below. If you projected the atom into one of those planes, it would be exactly in the middle of 3 atoms.

This position is the center of the equilateral triangle. If you're a big-time nerd and you already know how to calculate the centroid of an equilateral triangle, keep reading.

► **Otherwise, click this button.**

Now we can make another triangle, between d , $\frac{c}{2}$, and a .

$$(d)^2 + \left(\frac{c}{2}\right)^2 = a^2$$

$$\left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 = a^2$$

Which means that

$$c = \sqrt{\frac{8}{3}} a$$

Or

$$\frac{c}{a} \approx 1.633$$

And remembering that $a = 2r$,

$$c = 4\sqrt{\frac{2}{3}}$$

Now that we have a and c , we can calculate the **volume** of the hexagonal unit cell.

Hexagonal Close-Packed Unit Cell Volume

The hexagonal unit cell is just a hexagonal prism. You can google or memorize the answer quite easily, but in a test you might get extra points for deriving the result yourself.

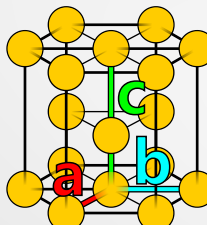
► **Click here to see one method.**

$$Volume_{HCP\ cell} = \frac{3\sqrt{3}}{2}a^2c$$

and using $c = \sqrt{\frac{8}{3}}a$ and $a = 2r$,

$$Volume_{HCP\ cell} = 24\sqrt{2}r^3$$

Volume of a Hexagonal Prism



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

Hexagonal Close-Packed
Open Visualization

Area of Triangle
= $\frac{1}{2}$ Base * Height = $\frac{a}{2} \sqrt{a^2 - \left(\frac{a}{2}\right)^2} = \frac{\sqrt{3}}{4}a^2$

Hexagon made of
6 triangles

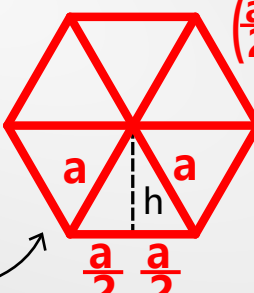
$\left(\frac{a}{2}\right)^2 + h^2 = a^2$

Area of Hexagon = $\frac{3\sqrt{3}}{2}a^2$

Volume of unit cell = $c \frac{3\sqrt{3}}{2}a^2$

Volume of hexagonal prism
= Area of **hexagon**
x **height** of prism

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



Volume of HCP Unit cell

$= 24\sqrt{2}r^3$

Now that we know the volume of the HCP unit cell, we can calculate it's APF!

Hexagonal Close-Packed Atomic Packing Fraction

The hard part is behind us. The atomic packing fraction (APF) is just the amount of atom inside the unit cell, compared to the overall size of the unit cell.

For the HCP cell, there are 12 corner atoms. Each corner atom has $\frac{1}{6}$ of its volume inside the unit cell. To visualize this, imagine that you joined many unit cells together. Each corner atom would be shared between 6 other cells, so it contributes $\frac{1}{6}$ to each.

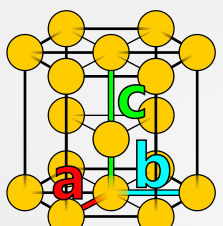
There are 2 atoms on the face, which each contribute $\frac{1}{2}$ of their volume.

There are 3 atoms in the center, which fully contribute their volume to the unit cell.

Altogether, that's 6 atoms per unit cell!

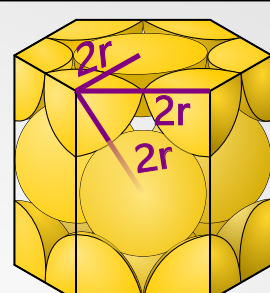
We know the volume of a sphere and we already calculated the volume of the unit cell, so

$$APF_{HCP} = \frac{\left(\frac{12}{6} + \frac{2}{2} + \frac{3}{1}\right) \frac{4}{3}\pi r^3}{24\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}} \approx 74\%$$



Hexagonal Close-Packed Open Visualization

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



12 atoms on the corners, with $\frac{1}{6}$ of their volume inside the unit cell **(2)**

+ **3 atoms** inside the cell, with **100%** of their volume inside the unit cell **(3)**

+ **2 atoms** on the faces, with $\frac{1}{2}$ of their volume inside the unit cell **(1)**

= 6 atoms per unit cell

$APF = \frac{\text{Volume of atoms}}{\text{Volume of unit cell}}$

Volume of atoms = $6 \cdot \frac{4}{3}\pi r^3$

Volume of unit cell = $24\sqrt{2}r^3$

For HCP

$APF = \frac{\pi}{3\sqrt{2}} = 74\%$

Final Thoughts

That's it! You've learned how to calculate the lattice parameters and atomic packing fraction for simple cubic (SC), body-centered cubic (BCC), face-centered cubic (FCC), and hexagonal close-packed (HCP) crystal systems.

Remember, APF is just the volume of the atoms within the unit cell, divided by the total volume of the unit cell. You use this to calculate the APF of *any* crystal system, even if it's non-cubic or has multiple kinds of atoms!

Brandon

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