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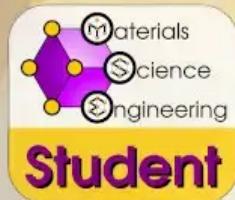
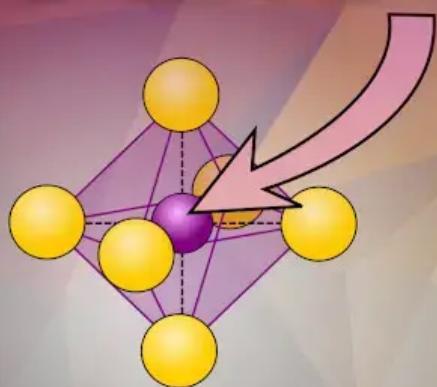
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## Interstitial Sites: Size, Types, Applications, And Calculations

# Interstitial Sites Types and Size



An important concept in crystallography is the idea of “interstitial sites,” which may also be called interstitial voids. They allow interstitial defects to occur. These sites exist in the

spaces between atoms, and you can actually calculate their size and position with simple geometry.

In this article, I'll explain how to perform these calculations, as well as the real-world differences that interstitial sites can make.

## Outline

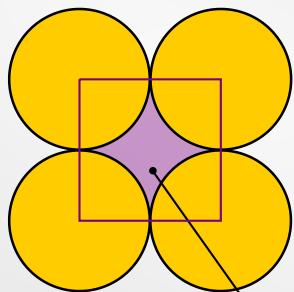
- What are Interstitial Sites?
- Why are Interstitial Defects Important?
- 4 Types of Interstitial Sites
- Interstitial Sites in FCC
- Interstitial Sites in BCC
- Interstitial Sites in HCC
- Interstitial Sites in Simple Cubic
- Interstitial Carbon in Steel
- Final Thoughts
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## What are Interstitial Sites?

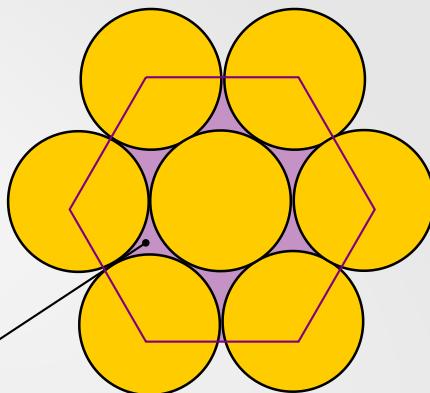
[Check out this article if you would like a basic introduction to crystallography](#), but the main fact you need to know is that crystals are any material made of atoms that repeat in a certain pattern.

If you have any pattern which doesn't fill space completely (and we model atoms as spheres that can never fill space completely), you end up with gaps.

## Square

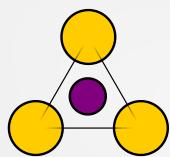


## Hexagon

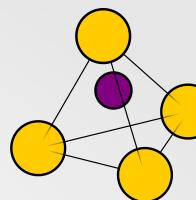


The empty spaces between atoms arranged in square are larger than those between atoms arranged in hexagon

Interstitial sites are empty spaces in a crystal lattice. Depending on the number of atoms surrounding that empty space, the interstitial site can be designated as **triangular** (3), **tetrahedral** (4), **octahedral** (6), or **cubic** (8).

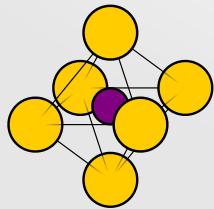


**Triangular**  
3 neighbors

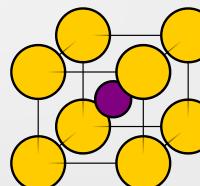


**Tetrahedral**  
4 neighbors

## 4 Types of Interstitial Sites



**Octahedral**  
6 neighbors



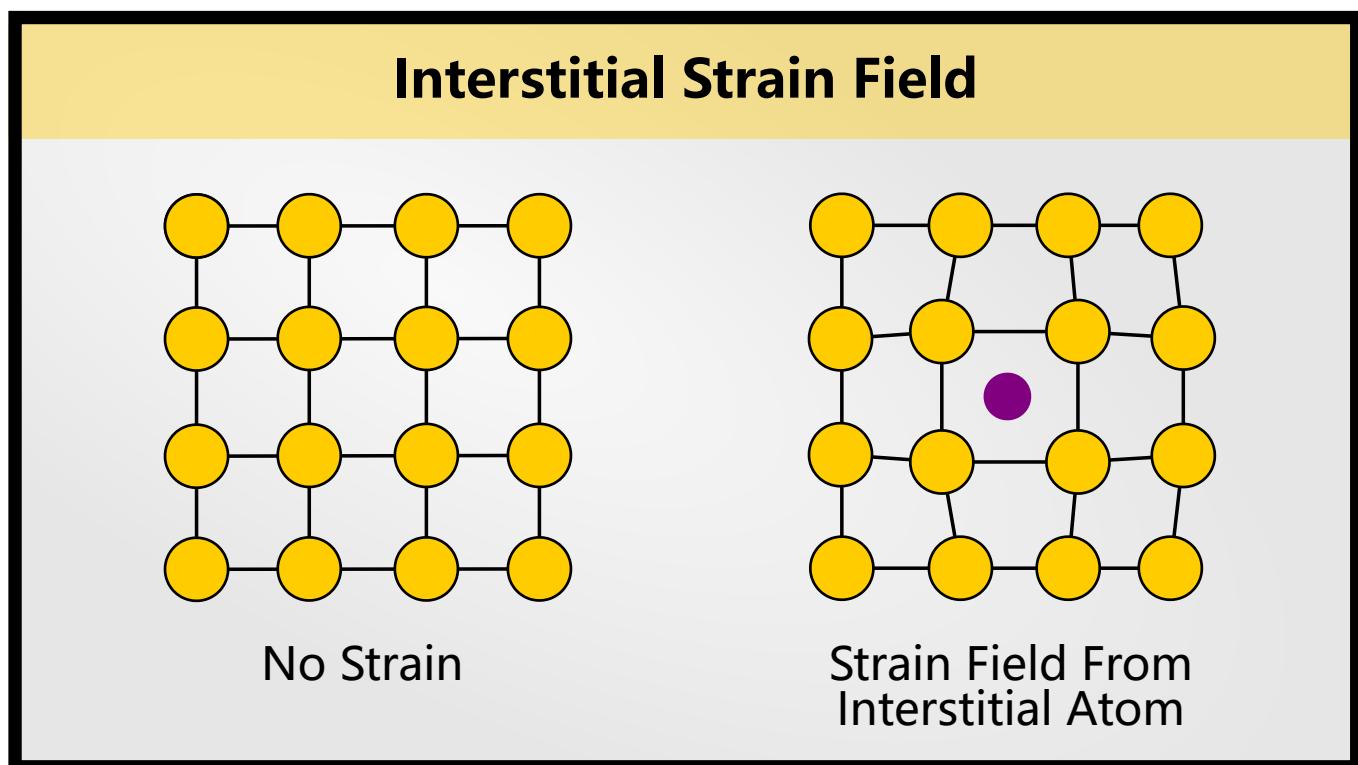
**Cubic**  
8 neighbors

Each interstitial site is empty in a perfect crystal, but since these are the regions in the crystal with the most empty space, imperfect crystals have an occasional atom in these sites.

## Why are Interstitial Defects Important?

When the interstitial site is not empty, it is considered an “interstitial defect.” **Defects allow some of the most important material properties**, such as ductility in metals. There are many kinds of crystal defects (besides interstitial defects) such as grain boundaries, vacancies, and dislocations.

Interstitial defects usually happen when a small atom fills the interstitial site of a larger atom’s crystal structure. Usually, this strains the crystal lattice and increases the strength of a metal. There are entire alloys based on this principle, called interstitial solid solution alloys.



The most famous example of an interstitial solid solution is when carbon rests in interstitial sites of iron—this is **steel**. If you know anything about metallurgy, you should know that steel is one of the most important materials in the world—mostly because of the way metallurgists can make its phases interact. The strongest phase of steel, *martensite*, exists because of carbon’s interaction with iron’s interstitial sites.

For now, I should explain more about how to perform calculations with interstitial sites. However, near the end of this article I will explain how martensite arises from the difference in interstitial size between FCC and BCC iron.

## 4 Types of Interstitial Sites

There are 4 standard types of interstitial sites, categorized by the number of surrounding atoms.

1. triangular
2. tetrahedral
3. octahedral
4. cubic

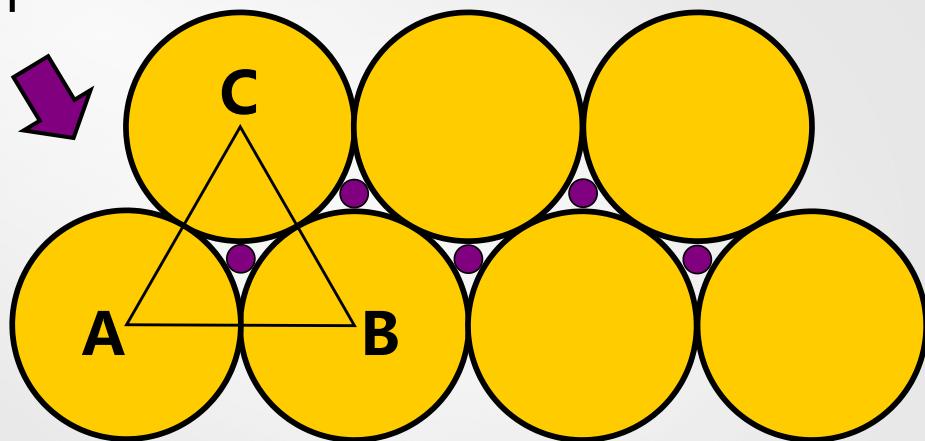
These 4 types of interstitial sites can be derived using the simple hard sphere model.

However, atoms are not perfect spheres, so interstitial atoms can sometimes be in other configurations, especially with complex crystal structures that may involve atoms of multiple sizes or asymmetrical interstitial sites.

A **triangular interstitial site** has 3 surrounding atoms. All 3 atoms, and the interstitial site, are in the same plane.

## Triangular Interstitial Sites

Triangular interstitial site between 3 atoms located in the same plane



## Calculating The Distance To The Center of an Equilateral Triangle

$$|AB|=|AC|=|BC|=a$$

$$|A'B| = \frac{a}{2}$$

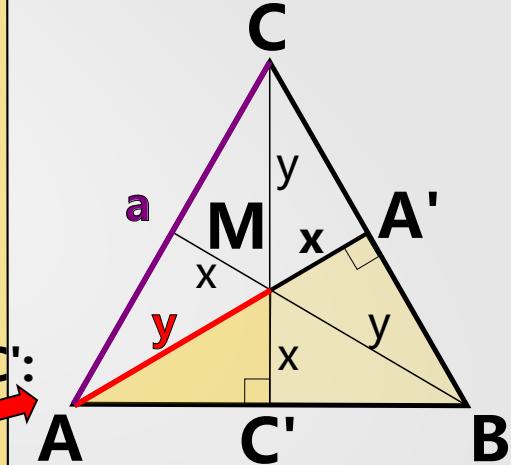
Pythagorean Theorem for  $\triangle ABA'$ :

$$|AB|^2 = |AA'|^2 + |A'B|^2$$



$$|AA'| = \frac{a\sqrt{3}}{2}$$

$$\text{Also, } |AA'| = x + y \quad \Rightarrow \quad x = \frac{a\sqrt{3}}{2} - y$$



Pythagorean Theorem for  $\triangle AMC'$ :

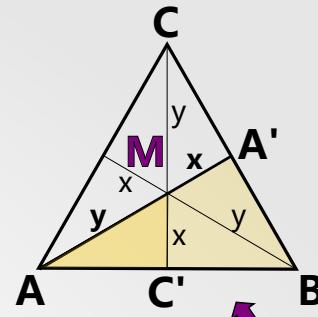
$$y^2 = \left[\frac{a}{2}\right]^2 + \left[\frac{a\sqrt{3}}{2} - y\right]^2 \quad \Rightarrow \quad y = \frac{a\sqrt{3}}{3}$$

## Calculating The Size of Triangular Interstitial Site

Since  $|AM| = y$ , and  $y = r + R$

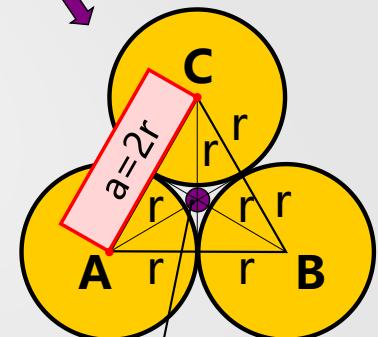
$$y = \frac{a\sqrt{3}}{3} \quad \Rightarrow \quad r + R = \frac{a\sqrt{3}}{3}$$

Also,  $a = 2r$ , hence:  $r + R = \frac{2r\sqrt{3}}{3}$



Triangular Interstitial Site Radius

$$R = r\left(\frac{2\sqrt{3}}{3} - 1\right)$$



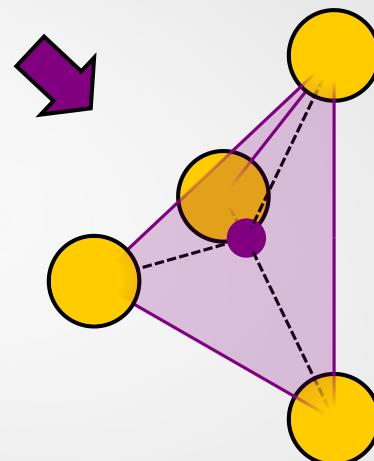
Interstitial Site Radius, R

A **tetrahedral interstitial site** has 4 surrounding atoms. These 4 atoms take the shape of a tetrahedron (4 equally spaced corners).

One simple way to imagine a tetrahedron is to take a cube (8 corners) and choose any 4 corners that are the maximum distance from each other.

## Tetrahedral Interstitial Sites

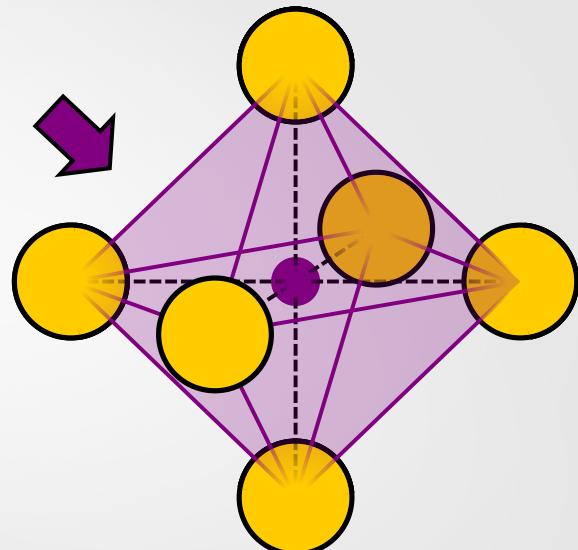
Tetrahedral interstitial site between 4 atoms



An **octahedral interstitial site** sits in the middle of 6 atoms. This “octahedral” shape looks as if you stuck 2 pyramids together at the base. The shape overall has 8 faces, which is where the “octahedral” name comes from.

## Octahedral Interstitial Sites

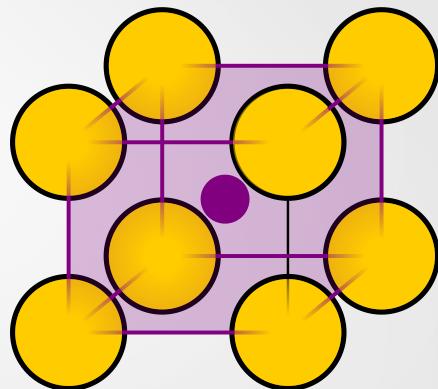
Octahedral interstitial site between 6 atoms



A **cubic interstitial site** is in the center of 8 atoms, which form a cube. The site is in the same spot as the center atom in a body-centered cubic (BCC) crystal.

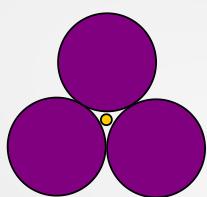
# Cubic Interstitial Sites

Cubic interstitial site  
between 8 atoms

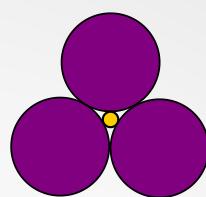


Although I've listed 4 types of interstitial sites, only tetrahedral and octahedral are important for most materials. That's because different interstitial sites have a different size compared to the surrounding atoms.

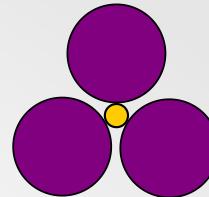
If you know how to calculate the anion-cation radius rules, calculating the regular atom-interstitial atom radius rules is identical ... *except* that interstitials don't really affect the bonding of the primary atoms, because there are so few.



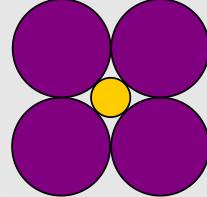
Cation too small:  
CN=3 unstable



Cation barely touches anion  
CN=3 stable

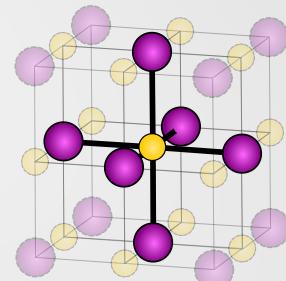


Cation more than touches anion  
CN=3 still stable



Cation barely touches anion  
CN=4 now stable

$$\frac{r_{\text{Na}^+} = 116 \text{ pm}}{r_{\text{Cl}^-} = 167 \text{ pm}} = 0.69$$



As you can see, triangular interstitial sites require extremely small atoms, and it's not really useful for most metals. For reference, hydrogen's atomic radius ( $0.53\text{\AA}$ ) is about  $\frac{1}{3}$  of iron's atomic radius ( $1.56\text{\AA}$ ), so even hydrogen is too small for triangular interstitial sites in iron [1].

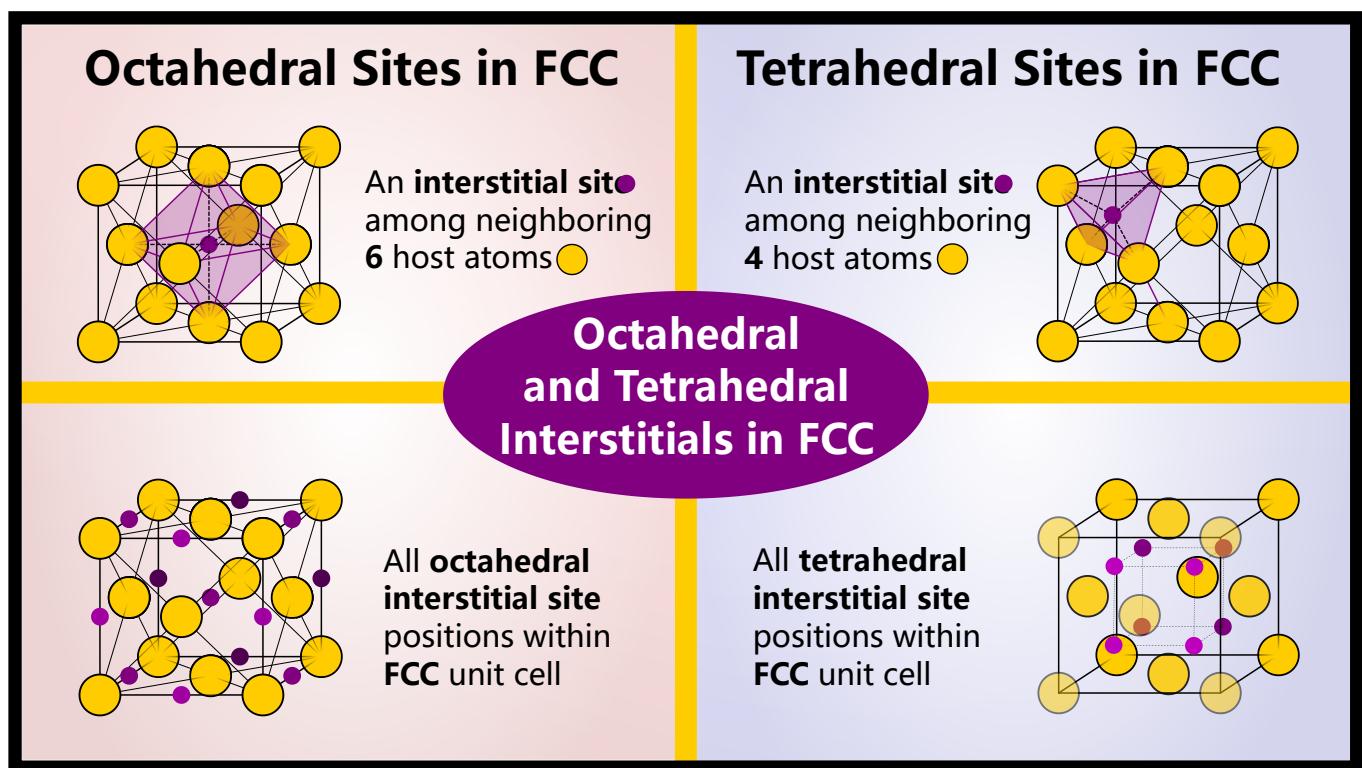
Likewise, a cubic interstitial site can be almost as big as the regular atom. Any crystal which has cubic interstitial sites (such as the simple cubic, or alpha-Po structure) are rare because they "waste" a lot of space.

Although cubic and triangular interstitial sites are too large and too small for most applications, tetrahedral and octahedral sites play an important role in materials science.

In the following sections, I'll calculate the size, number, and positions of octahedral and tetrahedral sites for the common crystal structures: FCC, BCC, HCP, and SC.

## Interstitial Sites in Face-Centered Cubic

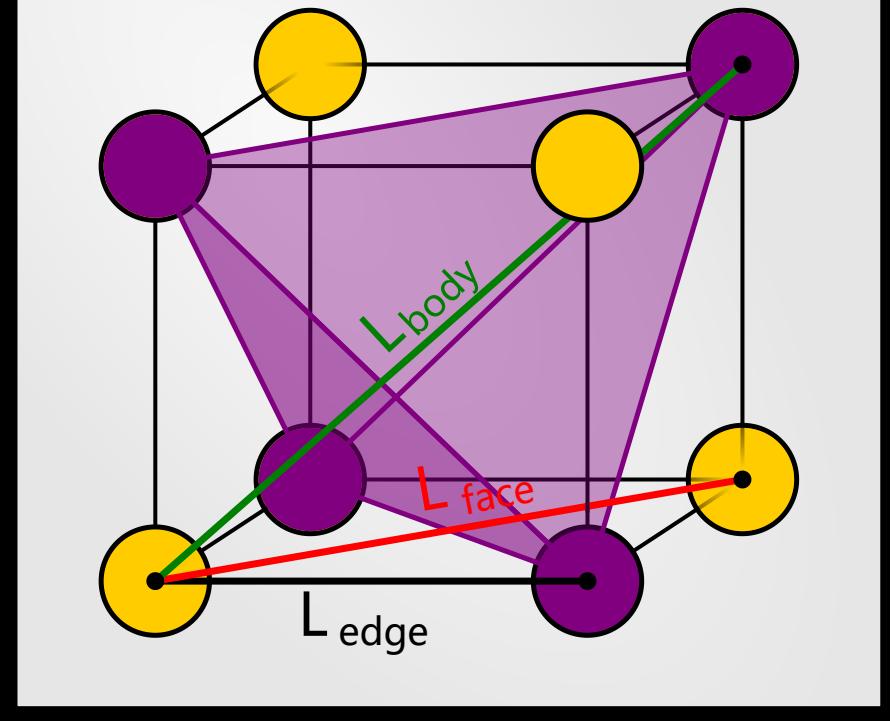
The FCC crystal has 8 tetrahedral sites and 4 octahedral sites.



Let's calculate the size of those interstitial sites ( $R$ ), compared to the size of an atom ( $r$ ). I'll start with the FCC tetrahedral void.

Remember, an easy way to do geometry involving tetrahedrons is to imagine that they are a cube that is missing half of its corners, like this.

# Tetrahedron Within a Cube



As you may know, the atom that sits in the center of a cube can touch the atoms at all 8 corners. That means that the corner-to-center distance, or  $\frac{1}{2}$  of the body diagonal will be the radius of the interstitial site + the radius of the atom.

To start, let's use this “imaginary cube” geometry to determine the corner-to-center distance.

Let's call the length of one cube edge  $L_{edge}$ . (If you're following the pictures below, I labelled the corners with letters). What we're looking for is the length of the body diagonal,  $L_{body}$ .

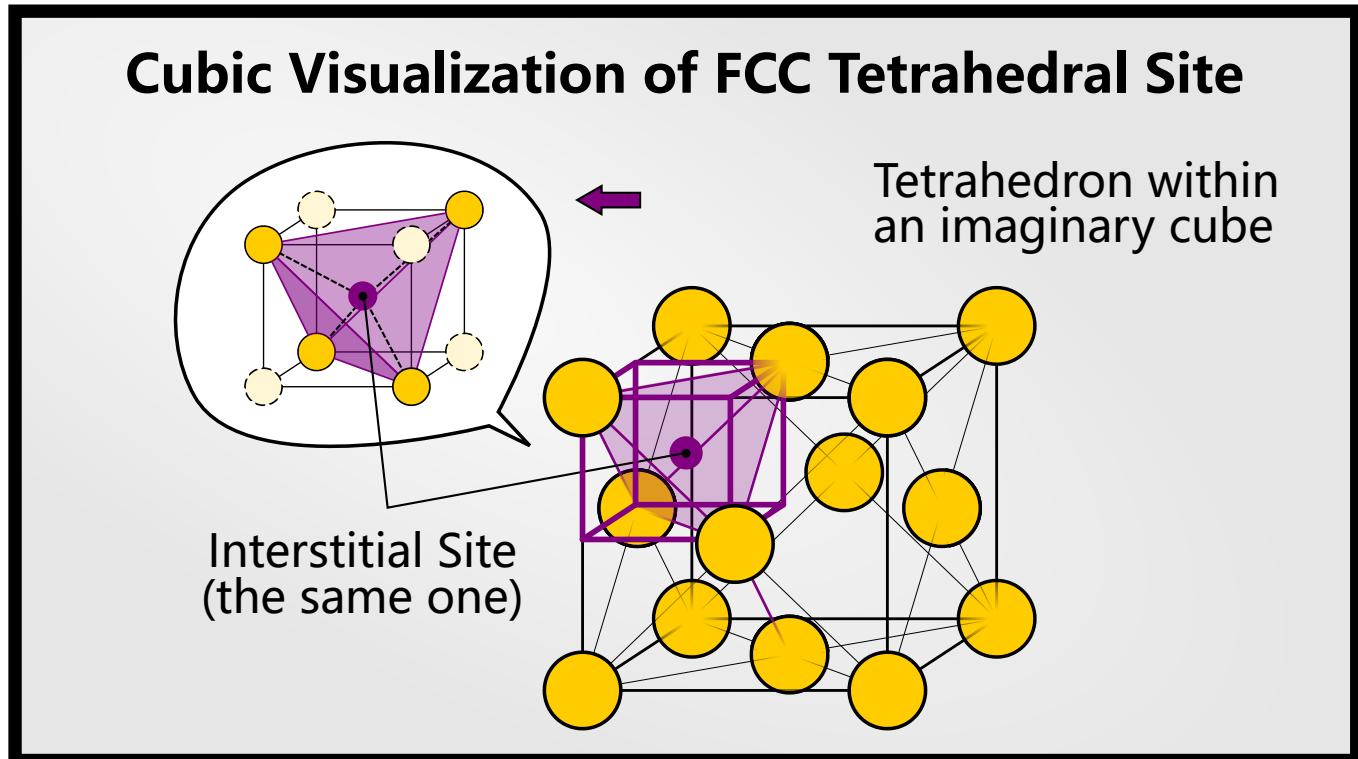
You can solve this directly with the 3D distance formula, or just use the pythagorean theorem in 2 steps:

First, let's find the length of the face diagonal,  $L_{face}$ . We know that  $(L_{edge})^2 + (L_{edge})^2 = (L_{face})^2$ . Rearranging tells us that  $L_{face} = \sqrt{2} \cdot L_{edge}$ .

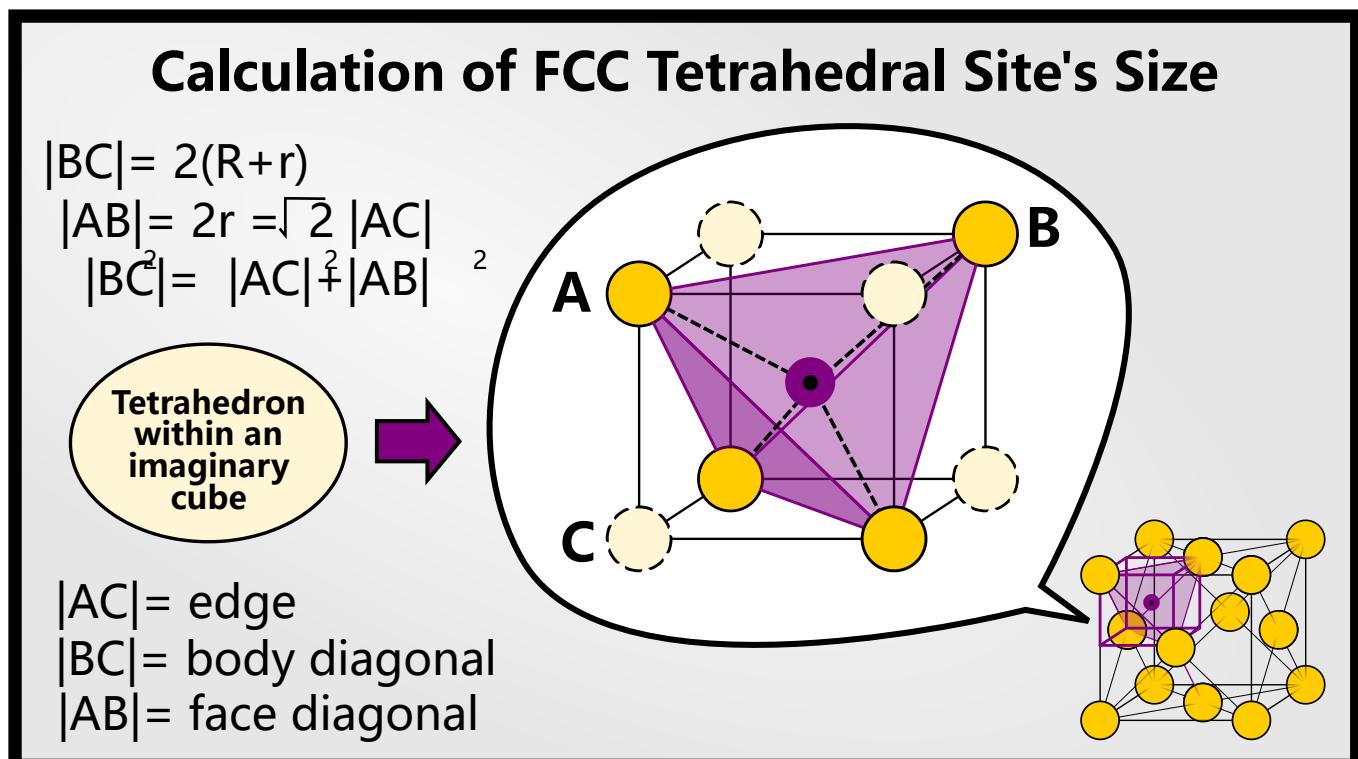
Now we can set up a 2nd pythagorean theorem, with  $(L_{edge})^2 + (L_{face})^2 = (L_{body})^2$ . Rearranging this gives us  $L_{body} = \sqrt{3} \cdot L_{edge}$ .

If we know the length of the body diagonal, then the distance from the corner to the center is half of that, or  $\frac{\sqrt{3}}{2}$  times the edge length.

Now we need to figure out the edge length, by putting our cube on top of the tetrahedral interstitial site.



In FCC, the tetrahedral edge length will be the distance between face-centered atoms. Since this is the close-packed direction, this distance is  $2r$ . When translating from the tetrahedron to our imaginary cube, the tetrahedron edge length becomes the cubic face diagonal.



So, we know that  $L_{face} = 2r$ . Earlier, we proved that  $L_{face} = \sqrt{2} \cdot L_{edge}$ , so  $L_{edge} = \frac{2r}{\sqrt{2}}$ .

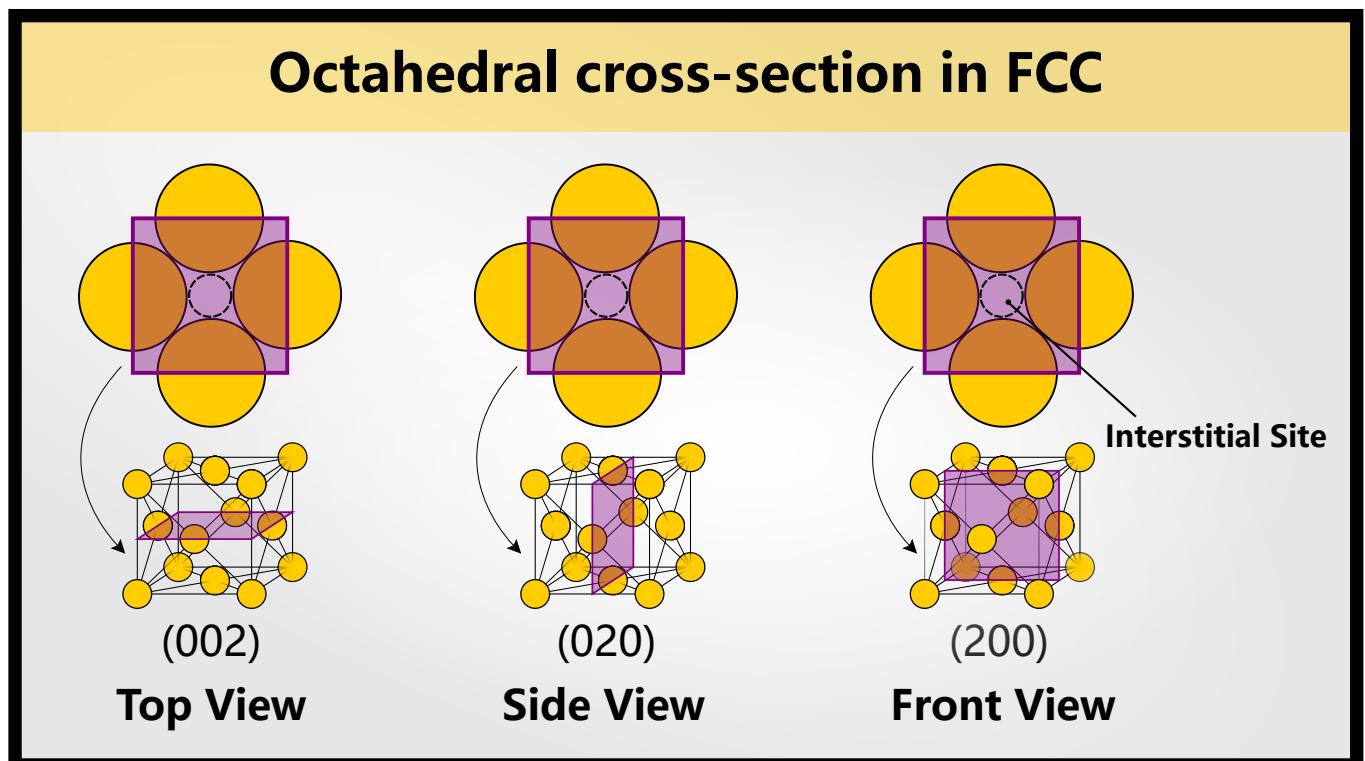
Plugging this back into the pythagorean theorem and we find that the  $(L_{body})^2 = 4r^2 + 2r^2$ .

$$2(r + R) = \frac{\sqrt{6}}{2} \cdot r$$

and finally, the radius  $R$  of the interstitial atom compare to the regular atom is:

$$R = r(\frac{\sqrt{6}}{2} - 1) \approx 0.2247r$$

Calculating the FCC octahedral interstitial sites is more straightforward than the tetrahedral sites. Whether we view the FCC cell from the top, front, or side, the 2D projection looks the same:

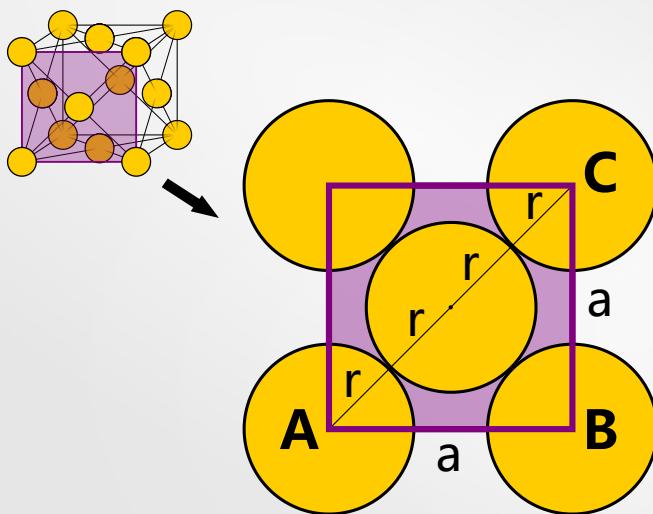


To calculate this interstitial size, we'll first calculate the size of a circle within that 2D plane. Then, we'll add the 3rd dimension. Let's view the FCC cell from the top—this is the (002) plane if you understand Miller Indices.

We have 4 atoms that make a square, with some space in the center. The diagonal across this square is the same as the edge length of the FCC cell. If you remember, for FCC  $a = 2\sqrt{2}r$ . If you don't remember, let's prove this again.

Since this is the close-packed plane, each circle on the corner of our square must touch another circle. The edge length of our cube is therefore  $2\sqrt{2}r$ .

## Edge Length (Lattice Parameter) in FCC



$$|AC| = 4r = \text{face diagonal}$$

$$|AB| = |BC| = a = \text{edge}$$

Pythagorean Theorem:

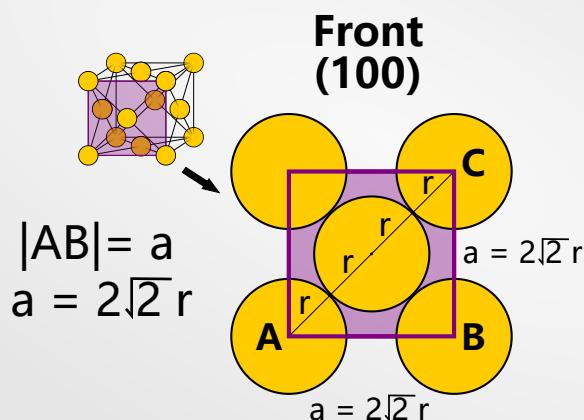
$$|AB|^2 + |BC|^2 = |AC|^2$$

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

$$a = 2\sqrt{2}r \text{ Edge Length}$$

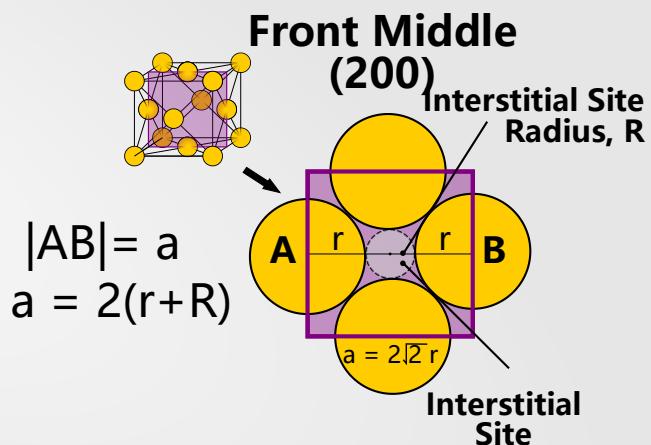
We know that the distance from one atom to the center is  $r + R$ , and we can use Pythagorean's theorem to put that in terms of the cube edge.

## Octahedral Interstitial Site Radius in FCC



$$|AB| = a$$

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



$$|AB| = a$$

$$a = 2(r+R)$$

$|AB|$  is the same distance in both pictures!

$$2(r+R) = 2\sqrt{2}r \rightarrow (r+R) = \sqrt{2}r \rightarrow R = r(\sqrt{2}-1) \text{ Interstitial Site Radius}$$

$$2(r+R) = 2 \cdot \sqrt{2}r$$

$$2R = 2 \cdot \sqrt{2}r - 2r$$

$$R = (\sqrt{2} - 1)r$$

This tells us the maximum radius of the interstitial size within that plane. However, we need to check the size in the 3rd dimension, height. If you look at the FCC crystal from the front or side views, you notice that the cross section looks exactly the same. Everything is symmetrical, and you find the same value for R in every dimension.

So,  $R = (\sqrt{2} - 1)r \approx 0.4142$  just like we thought.

I make a point to emphasize this because the symmetry assumption is NOT true for BCC.

### **Total volume of interstitial sites in FCC crystals:**

$$V_{interstitials} = 8 \cdot \frac{4}{3} \cdot \pi \cdot (R_{tetrahedral})^3 + 4 \cdot \frac{4}{3} \cdot \pi \cdot (R_{octahedral})^3$$

where  $R_{tetrahedral} = (\frac{\sqrt{6}}{2} - 1)r$

and  $R_{octahedral} = (\sqrt{2} - 1)r$

### **The volume of an FCC cell is:**

$$V_{FCC} = a^3 = (2\sqrt{2}r)^3$$

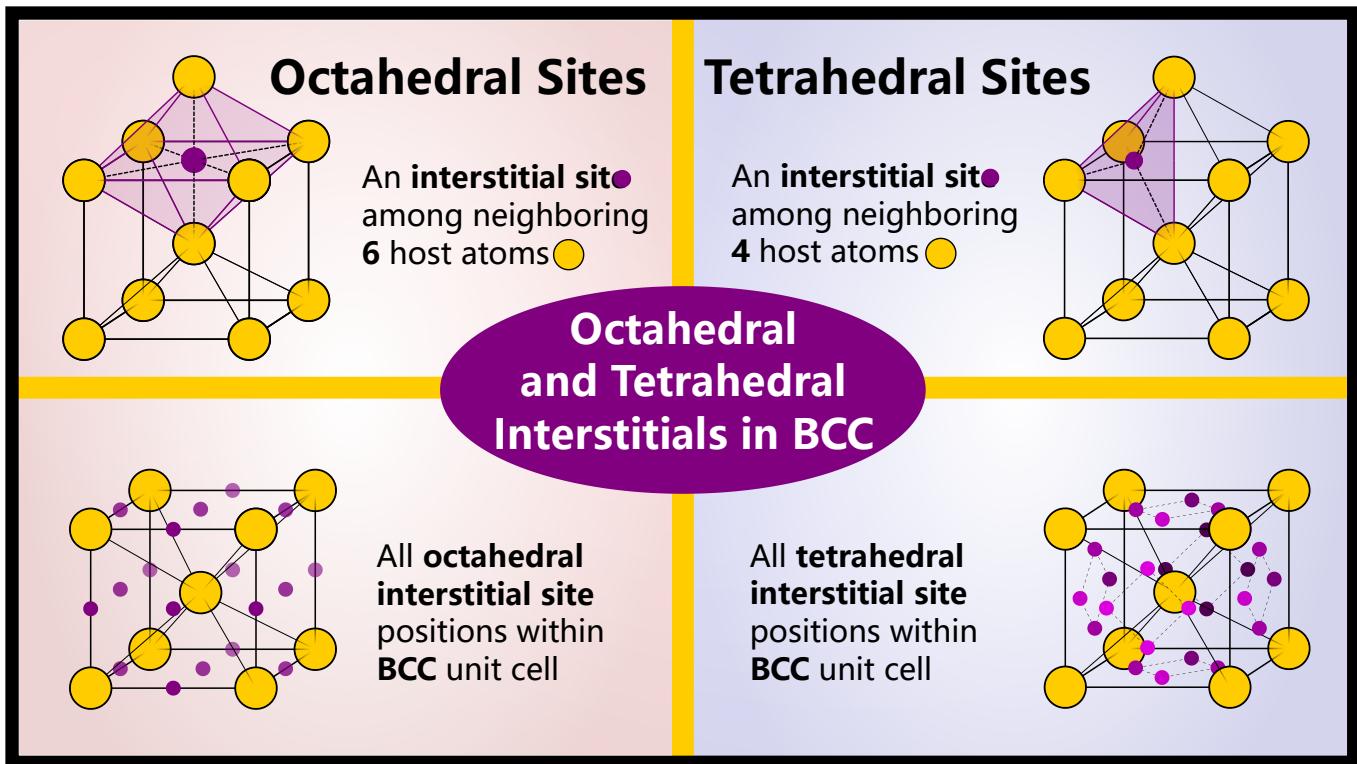
### **Hence, the fraction occupied by interstitial sites is:**

$$V_{interstitials} : V_{FCC} = 6.94\%$$

So an FCC crystal can fill **about 7%** of its volume with interstitial atoms! Of course, if an FCC crystal was really filled with so many interstitial atoms, the lattice parameter would definitely distort and it would change to a different crystal structure.

## **Interstitial Sites in BCC**

The BCC crystal has 12 tetrahedral sites and 6 octahedral sites.



Let's calculate the size of those interstitial sites, compared to the size of the atom, starting with the BCC tetrahedral void.

This calculation is similar to the FCC tetrahedral interstitial site, but slightly more complex because the tetrahedron is not completely symmetrical.

If you look at the tetrahedral site, 2 edges have a length equal to the BCC lattice parameter, and the other 4 edges have a length equal to half of the body diagonal.

## Tetrahedral Interstitial Site in BCC

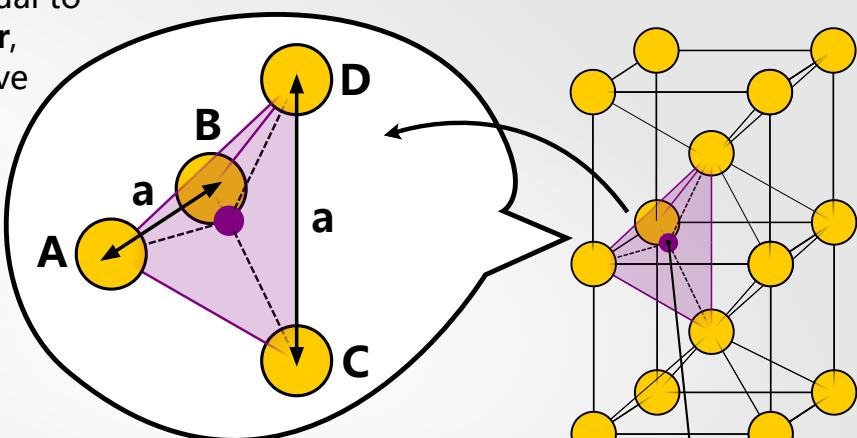
**2 edges** have a length equal to the BCC **lattice parameter**, and the other **4 edges** have a length equal to **half of the body diagonal**.

**Edge length "a" in BCC:**

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

$$|AB|=|DC|= a$$

$$|AC|=|BC|=|AD|=|BD|= 2r$$



Interstitial Site

These values are  $\frac{4r}{\sqrt{3}}$  and  $2r$ . If you'd like a proof for that, you can [check out the BCC section in my article about calculating the atomic packing factor](#).

Instead of transposing our tetrahedron on a cube, we'll now put it on a rectangular prism.

## Tetrahedral Interstitial in BCC: Rectangular Prism

**Imaginary Rectangular Prism**

$|AB|=|DC|= a$   
 $|AC|=|BC|=|AD|=|BD|= 2r$   
 $|BE| = \frac{a}{2}$

**Edge length "a" in BCC:**  $a = \frac{4r}{\sqrt{3}}$

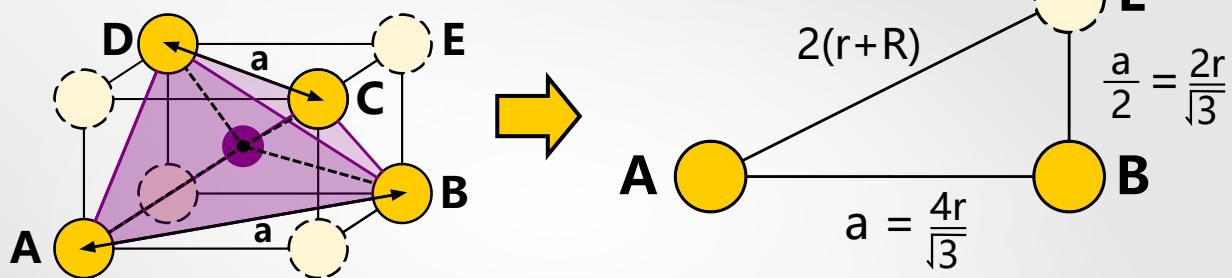
The body diagonal of this prism,  $L_{body}$ , is still  $r + R$ . And we can still use a series of Pythagorean theorems like we did for the FCC tetrahedral site, but this time I'll make sure that  $L_{face}$  is only made of the short edges, and  $L_{edge}$  considers the long edge, as labelled in the diagram above. You can switch the values however you like, but that's how I will label them in these diagrams.

You can also use the 3D distance formula, which says that the square of the body diagonal will be the sum of the squares of each edge length. It works out the same.

We need to put the imaginary rectangular prism back on the BCC cell, as you can see above, to understand the relationships between the tetrahedral edges and the atomic radii.

# Size of Tetrahedral Interstitial in BCC

## Imaginary Rectangular Prism



Pythagorean Theorem for  $\triangle ABE$ :

$$|AB|^2 + |BE|^2 = |AE|^2 \Rightarrow \left[\frac{4r}{\sqrt{3}}\right]^2 + \left[\frac{2r}{\sqrt{3}}\right]^2 = [2(r+R)]^2 \Rightarrow R = r\left(\frac{\sqrt{5}}{\sqrt{3}} - 1\right)$$

**Interstitial Site Radius**

As you can see,  $L_{face} = 2r$ , and  $L_{edge} = \frac{4r}{\sqrt{3}}$ .

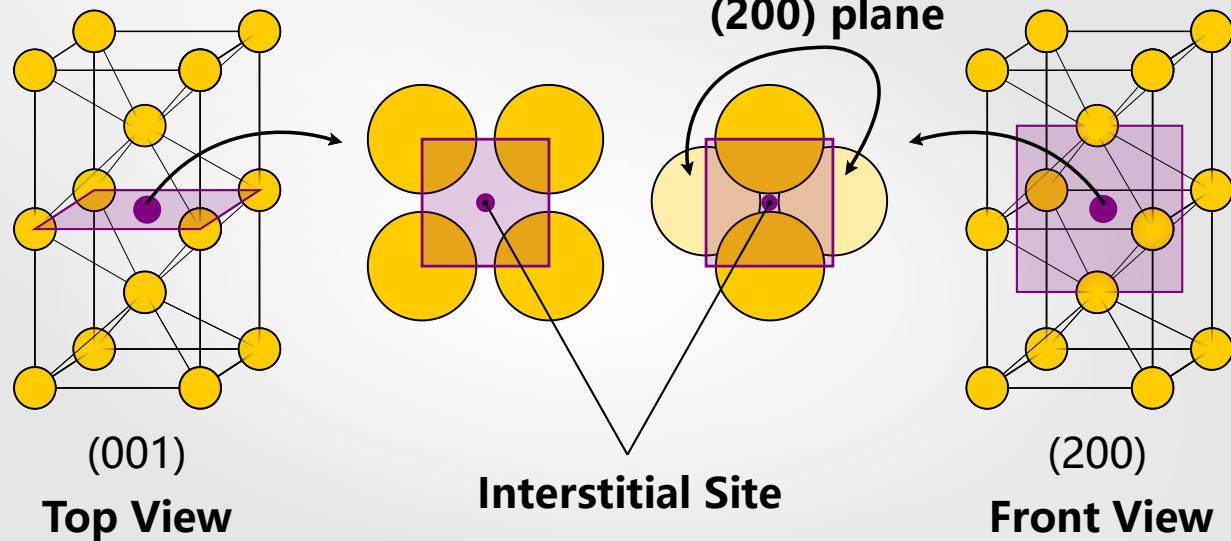
$$(2r + 2R)^2 = \left(\frac{4r}{\sqrt{3}}\right)^2 + \left(\frac{2r}{\sqrt{3}}\right)^2$$

$$R = r\left(\frac{\sqrt{5}}{\sqrt{3}} - 1\right)$$

Calculating the BCC octahedral site sizes can be done similarly to FCC octahedral sites, but you have to be careful about the asymmetry.

If you look at the cell from the top view, you see a nice cube where the cube edges match the BCC edge lengths. However, if you look from the front or side view, the cube has *face diagonals* which match the BCC edge lengths.

# Octahedral cross-section in BCC



We can still project things into 2D, but we need to assess the top and front/side views separately. Let's start with the top view.

In this projection, you can see that the interstitial site falls in the center of a square, where each corner of the square has an atom. The edges of this square line up with the edges of the BCC cube, and you know that distance is  $\frac{4}{\sqrt{3}}r$ .

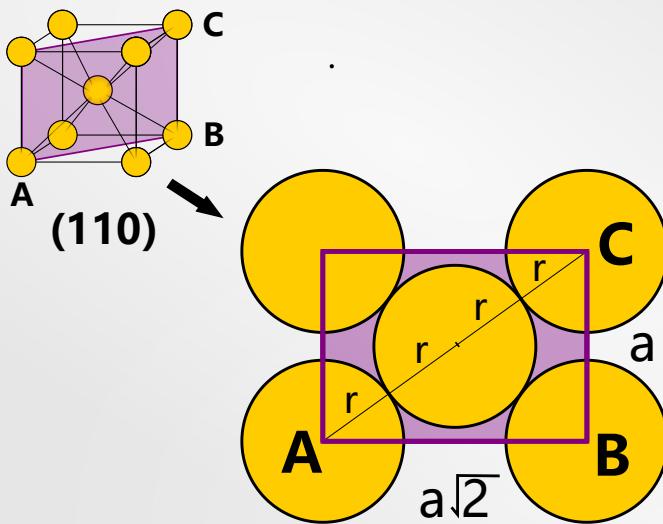
(If you *didn't* know that the BCC lattice parameter is  $a = \frac{4}{\sqrt{3}}r$ , [I once again recommend my article about calculating APF](#).)

The geometry using Pythagorean's theorem should be familiar by now. The face diagonal is  $2(r + R)$  and so  $(2(r + R))^2 = (\frac{4}{\sqrt{3}}r)^2 + (\frac{4}{\sqrt{3}}r)^2$ .

and finally that simplifies to  $R = r(\frac{\sqrt{8}}{\sqrt{3}} - 1)$

But remember, we're not done. Now we need to check the interstitial position in the 3rd dimension. The top and bottom atoms of the octahedron are the center atom in the BCC cell. In other words, the height of the octahedron is exactly the distance as the BCC lattice parameter,  $a = \frac{4}{\sqrt{3}}r$ .

## Edge Length (Lattice Parameter) in BCC



$$|AC| = 4r = \text{body diagonal}$$

$$|AB| = a\sqrt{2} = \text{face diagonal}$$

$$|BC| = a = \text{edge}$$

Pythagorean Theorem:

$$|AB|^2 + |BC|^2 = |AC|^2$$

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

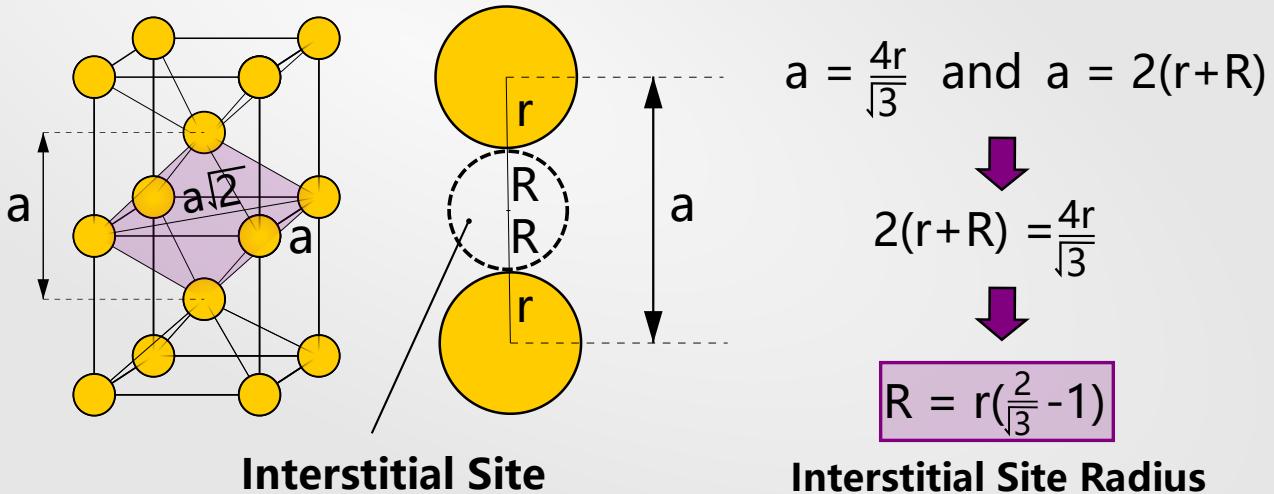
$$a = \frac{4r}{\sqrt{3}} \text{ Edge Length}$$

As you can see, that height is  $2(r + R) = \frac{4}{\sqrt{3}}r$

and rearranging for  $R$  gives  $R = (\frac{2}{\sqrt{3}} - 1)r$

## Octahedral Interstitial Site Radius in BCC

Since interstitial site radius is always limited by the **shortest distance** between atoms (and  $a < a\sqrt{2}$ ), then  $r+R+R+r = a$



$$a = \frac{4r}{\sqrt{3}} \text{ and } a = 2(r+R)$$

$$2(r+R) = \frac{4r}{\sqrt{3}}$$

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

**Interstitial Site Radius**

We need to compare the maximum values that we calculated for  $R$ , and  $(\frac{2}{\sqrt{3}} - 1)r$  is smaller than  $r(\frac{\sqrt{8}}{\sqrt{3}} - 1)$ . This means that the interstitial site could be larger if the top and bottom of the octahedral were farther apart.

The true maximum value for  $R$  is  $(\frac{2}{\sqrt{3}} - 1)r \approx 0.1547r$ .

## Total volume of interstitial sites in BCC crystals:

$$V_{interstitials} = 12 \cdot \frac{4}{3} \cdot \pi \cdot (R_{tetrahedral})^3 + 6 \cdot \frac{4}{3} \cdot \pi \cdot (R_{octahedral})^3$$

where  $R_{tetrahedral} = (\frac{\sqrt{5}}{\sqrt{3}} - 1)r$

and  $R_{octahedral} = (\frac{2}{\sqrt{3}} - 1)r$

## The volume of a BCC cell is:

$$V_{BCC} = a^3 = (\frac{4r}{\sqrt{3}})^3$$

**Dividing by the volume of the unit cell will give us the maximum volume fraction of interstitial sites in BCC.**

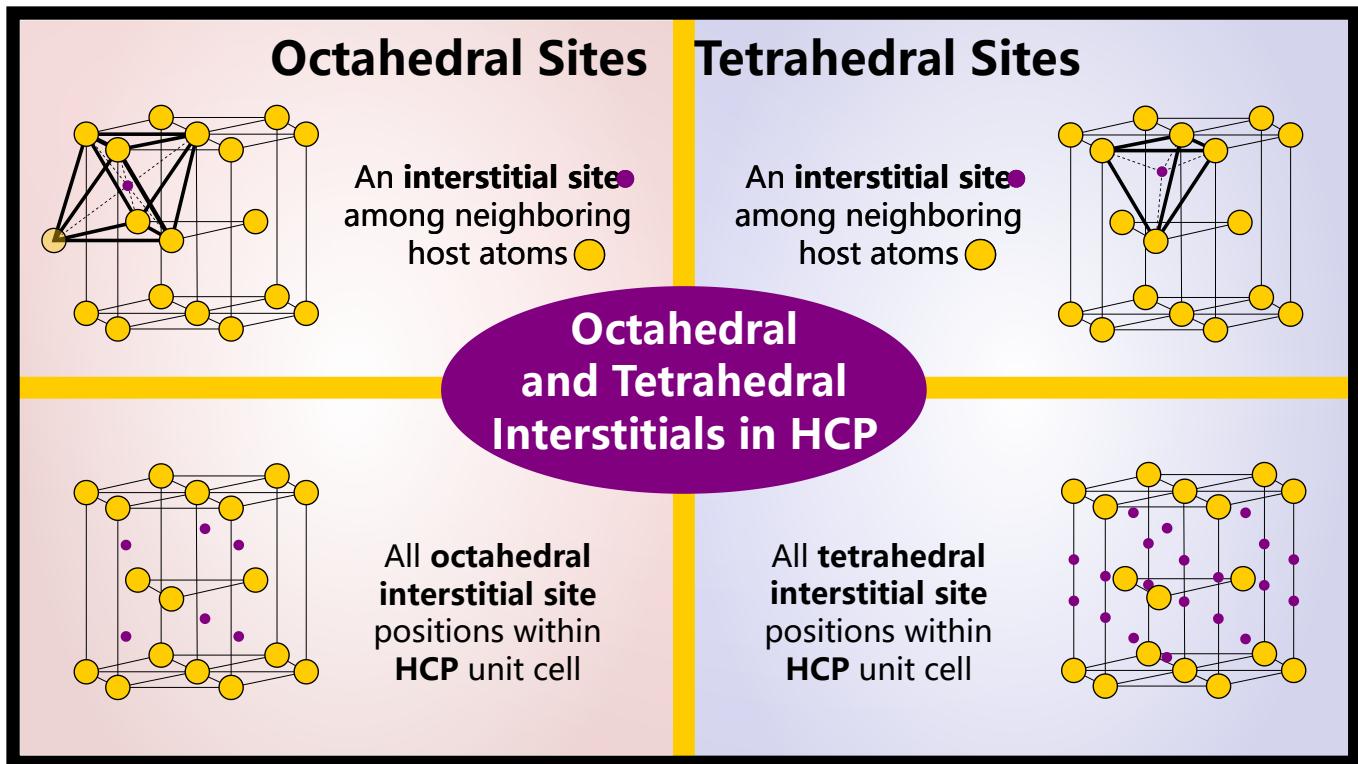
$$V_{interstitials} : V_{BCC} = 10.81\%$$

So BCC can have **about 11%** of its volume occupied by interstitial atoms. (Theoretically, not in reality).

Notice that this is greater than the total volume of FCC interstitial sites, which should make sense because FCC is atomically denser than BCC.

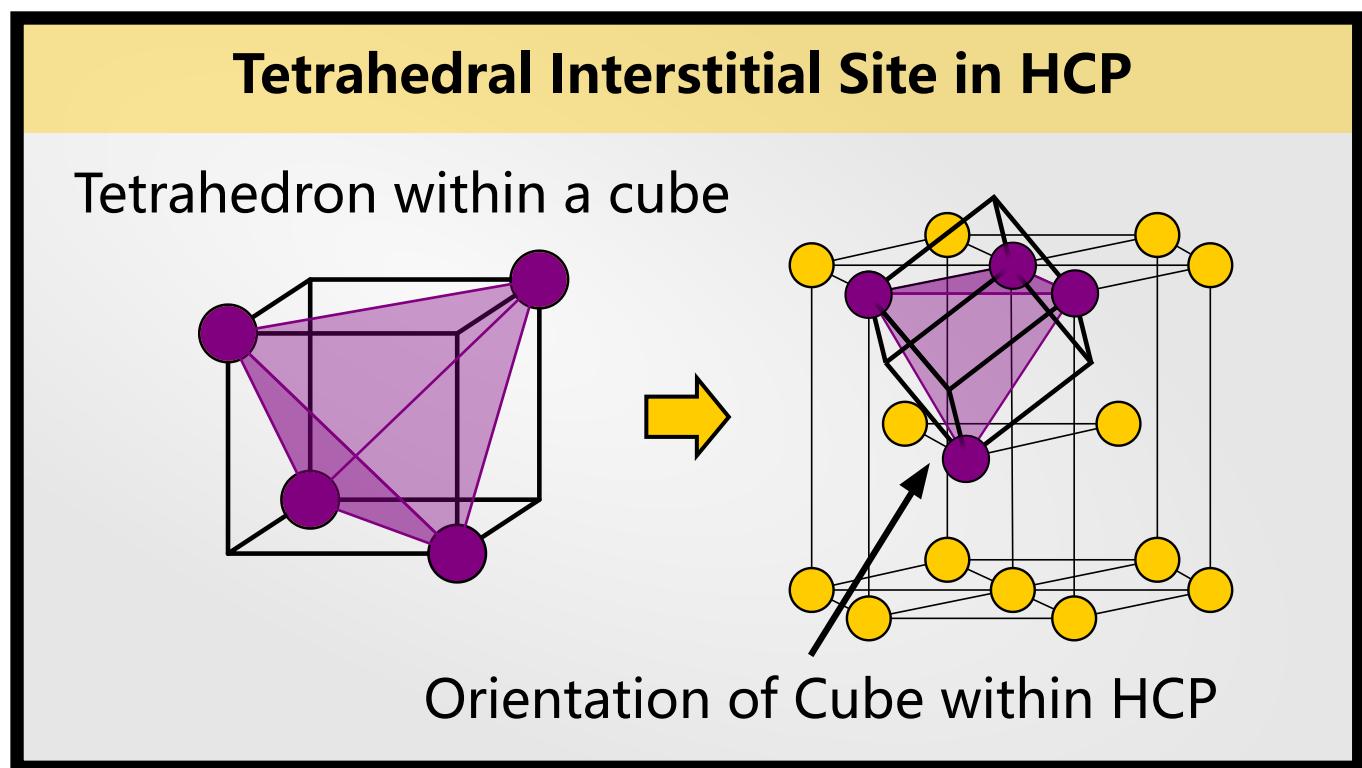
## Interstitial Sites in HCP

The HCP unit cell has 12 tetrahedral sites and 6 octahedral sites, which is exactly 50% more than the FCC sites. This shouldn't be a surprise, considering that both FCC and HCP are close-packed, and HCP is exactly 50% larger than FCC.



Calculating the tetrahedral and octahedral sites for HCP works out exactly like calculating them for FCC. Remember, the difference between FCC and HCP is stacking order, so all that's changed is the position of the interstitial sites within the stack.

For the tetrahedral site, we once again visualize the tetrahedron within an imaginary cube.

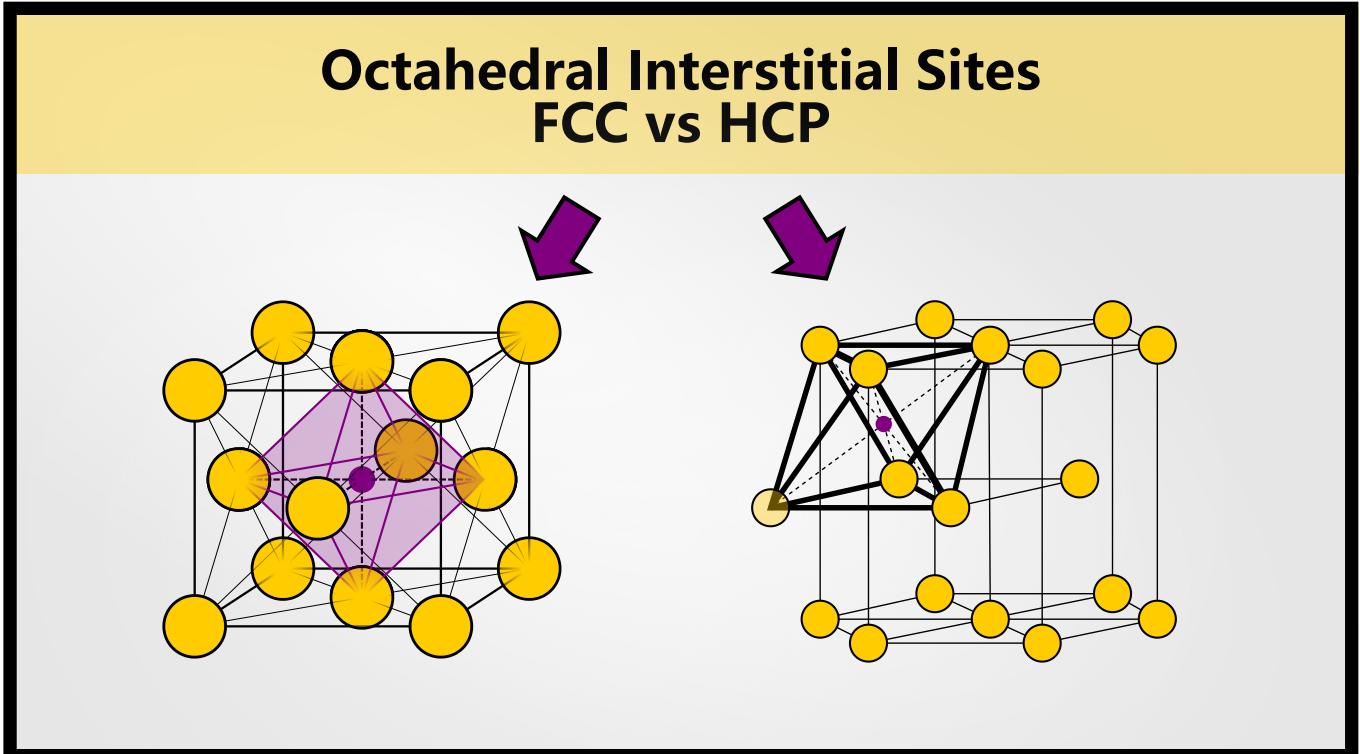


As you can see, the face diagonals of this cube are the close-packed direction and are therefore equal to  $2r$ . That means this tetrahedron is exactly the same as the tetrahedron in

FCC, so if you follow that derivation you end up with

$$R = r(\frac{\sqrt{6}}{2} - 1)$$

The HCP octahedral sites also have each edge length =  $2r$ , which is identical to the FCC octahedral sites

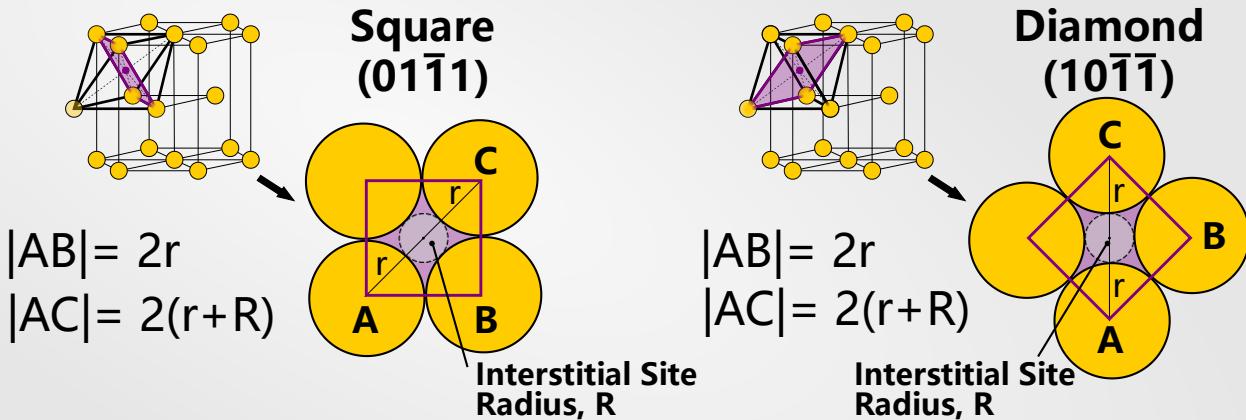


The geometry is the same, but I'll work it out again because I can't use some of the cubic shortcuts we did when calculating the size of FCC interstitial sites.

Let's start by looking at the square cross section. As we just discussed, each edge of this square has a length of  $2r$ . The space within the plane is  $(2(r + R))^2 = (2r)^2 + (2r)^2$ , which means  $R = r(\sqrt{2} - 1)$

We then need to consider the 3rd axis, the “height” of the octahedron. If we view the octahedron from the side, so it looks like a diamond, we see that both body diagonals are  $2(r + R)$ .

# Octahedral Interstitial Site Radius in HCP



$$\text{For } \triangle ABC: |AC|^2 = |AB|^2 + |AB|^2 \rightarrow |AC| = \sqrt{2} |AB|$$

$$2(r+R) = 2\sqrt{2} r \rightarrow (r+R) = \sqrt{2} r \rightarrow R = r(\sqrt{2}-1) \text{ Interstitial Site Radius}$$

This is obviously symmetric with the body diagonal when we looked through the other perspective, but let's keep going. We see that  $(r+R)^2 + (r+R)^2 = (2r)^2$ , and eventually we can reduce the "height" of the octahedron to  $r+R = \sqrt{2}r$ , and therefore  $R = r(\sqrt{2}-1)$ , in every perspective.

Thus,  $R = r(\sqrt{2}-1)$  is the true maximum radius for an octahedral interstitial in the HCP crystal.

**Total volume of interstitial sites in HCP crystals:**

$$V_{interstitials} = 12 \cdot \frac{4}{3} \cdot \pi \cdot (R_{tetrahedral})^3 + 8 \cdot \frac{4}{3} \cdot \pi \cdot (R_{octahedral})^3$$

$$\text{where } R_{tetrahedral} = \left(\frac{\sqrt{6}}{2} - 1\right)r$$

$$\text{and } R_{octahedral} = (\sqrt{2}-1)r$$

**The volume of an HCP cell is:**

$$V_{HCP} = S_{base} \cdot H = 6 \cdot \frac{1}{2} \cdot a \cdot \frac{a\sqrt{3}}{2} \cdot \frac{4\sqrt{2}}{\sqrt{3}} = 6 \cdot \frac{1}{2} \cdot 2r \cdot \frac{2r\sqrt{3}}{2} \cdot \frac{4\sqrt{2}}{\sqrt{3}} = 24\sqrt{2}$$

**Hence, the fraction occupied by interstitial sites is:**

$$V_{interstitials} : V_{HCP} = 6.94\%$$

Interstitial sites occupy exactly the same volume (6.94%) for FCC and HCP unit cells. That makes perfect sense since both crystal structures are close-packed with an atomic packing factor (APF) of 74%.

## Interstitial Sites in Simple Cubic

Simple cubic has one cubic interstitial site. As you can imagine, it's right in the center of the atom.

### Interstitial Site Radius in SC

$|AB| = a$   
 $|DC| = a$   
 $a = 2r$

**(001)**

$|AC| = a\sqrt{2}$   
 $|AD| = a\sqrt{3}$

**(110)**

$R = r(\sqrt{3}-1)$  **Interstitial Site Radius**

As you can probably guess by now, we can calculate the size of this interstitial site by realizing that the body diagonal is twice the radius of the atom and the interstitial site.

By the 3D distance formula or a couple applications of Pythagorean's theorem, you can see that the body diagonal is  $\sqrt{3}$  times the edge length of the cube. In the simple cubic crystal structure, the edge length is  $2r$ , so

$$2(r + R) = 2r\sqrt{3}$$

$$R = r(\sqrt{3} - 1)$$

**Total volume of interstitial sites in SC crystals:**

$$V_{interstitials} = \frac{4}{3} \cdot \pi \cdot (R_{cubic})^3$$

and  $R_{cubic} = (\sqrt{3} - 1)r$

**The volume of an SC cell is:**

$$V_{SC} = a^3 = (2r)^3$$

**Hence, the fraction occupied by interstitial sites is:**

$$V_{interstitials} : V_{SC} = 20.54\%$$

## Interstitial Carbon in Steel

A lot of steel's unique properties come from the fact that iron changes from BCC to FCC at high temperatures, and carbon has to move between those interstitial sites.

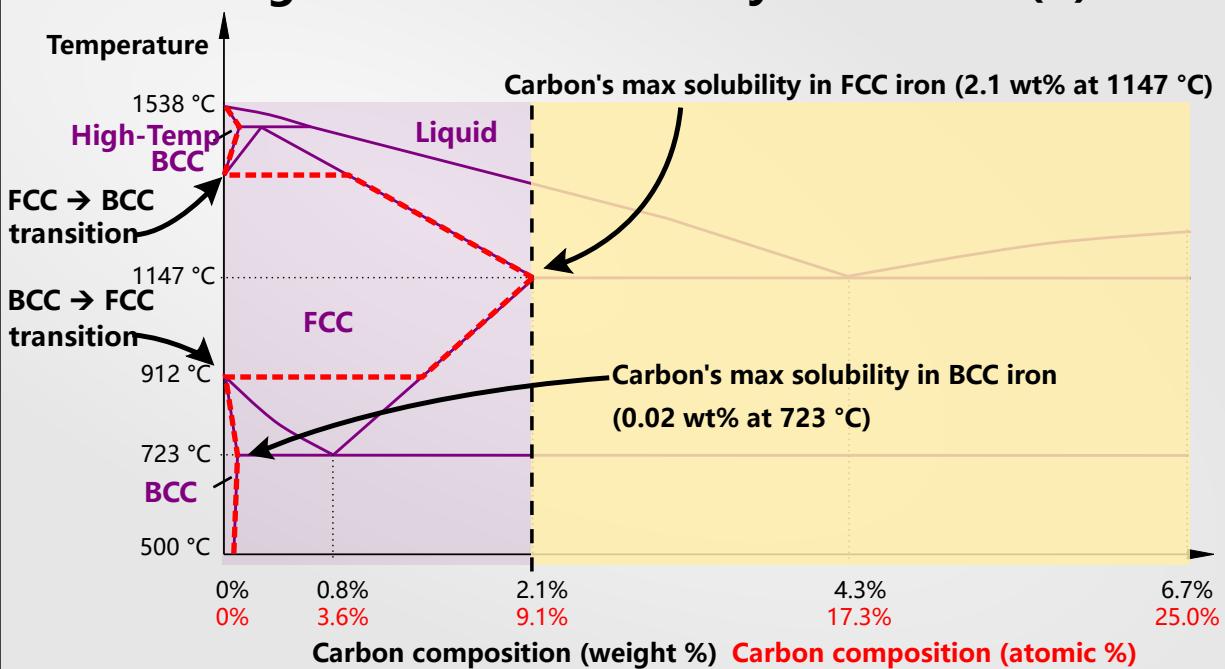
Carbon forms an **interstitial solid solution** when added to iron; the maximum concentration of carbon is about 2 wt%. The atomic radius of the **carbon** atom is much less than that for **iron: 0.071 nm** versus **0.124 nm** [2]. In other words, the carbon atom is 57% as large as the iron atom.

From a simple APF calculation, you should know that BCC has a larger total volume of interstitial space than FCC. Earlier, we proved that directly.

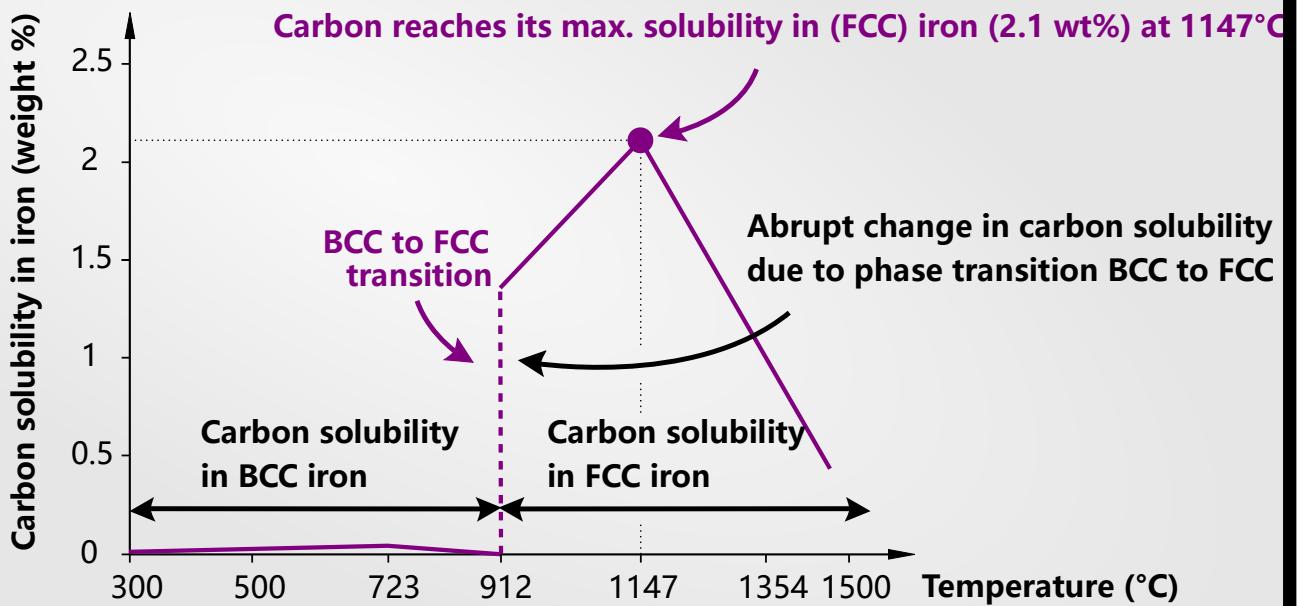
However, FCC has the largest interstitial site. FCC's largest interstitial site is octahedral, which is 41% of the atom size. BCC's largest interstitial size is tetrahedral, which is 29% of the atom size. As you can see, it's a lot easier to squeeze carbon into an interstitial site in FCC iron, compared to squeezing it in the smaller interstitial sites in BCC iron. This means that the solubility of carbon in iron is about 100 times higher for FCC than BCC!

As you heat up iron, it will change from BCC to FCC at 912°C. Suddenly, the metal will be able to absorb a lot more carbon from the atmosphere.

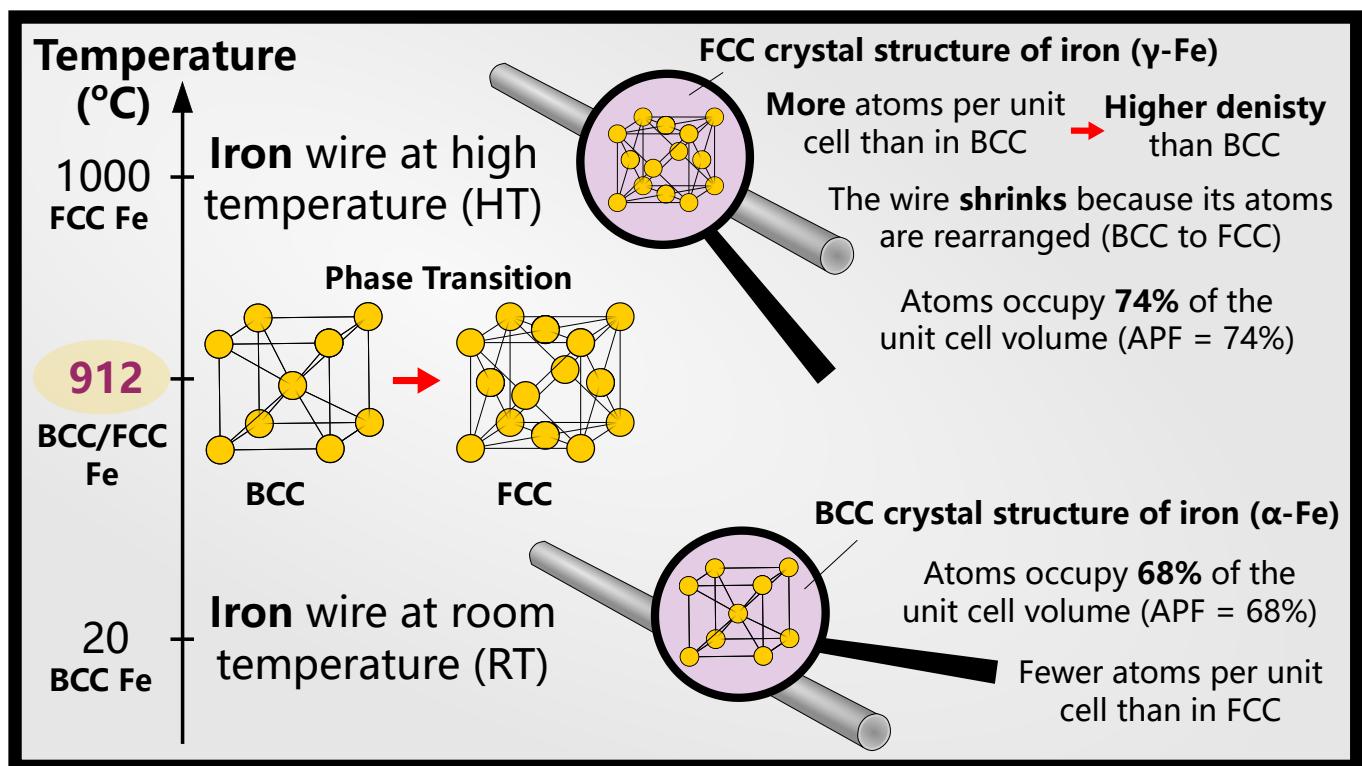
# Phase Diagram Shows Solubility of Carbon (C) in Iron (Fe)



## Carbon (C) Solubility in BCC and FCC Iron (Fe)



When you cool down the iron, the atoms want to shift back to BCC, but now there's too much carbon! If you cool it slowly, the carbon has time to get squeezed out and the iron can be BCC again. However, if you cool it quickly (quenching), then the carbon gets frozen in the interstitial sites and you end up with a distorted body-centered tetragonal structure.



I previously wrote an article about [quenching](#) (and tempering, a completely different process that is commonly confused with quenching), so be sure to check that out next!

## Final Thoughts

Although introductory materials science classes might spend only one day explaining interstitial sites, the topic is important for understanding advanced metallurgy, especially about steel. With simple geometry, you can calculate the size of an interstitial site for different crystal structures.

Crystal Structure	BCC	FCC	HCP	SC
<b>Octahedral Interstitial Site Radius</b>	0.155r	0.414r	0.414r	-
<b>Tetrahedral Interstitial Site Radius</b>	0.291r	0.225r	0.225r	-
<b>Cubic Interstitial Site Radius</b>	-	-	-	0.732r
<b>Fraction of a cell's volume occupied by interstitial sites</b>	10.81%	6.94%	6.94%	20.54%

# References and Further Reading

[1] [CrystalMaker](#)

[2] Callister W., Fundamentals of Materials Science and Engineering, John Wiley & Sons, Inc., 2001.

If you're reading this article as an introductory student in materials science, welcome! I hope you can find many other useful articles on this website. You may be interested in a related article I've written about [Atomic Packing Factor](#).

If you're reading this article because you're taking a class on structures, you may be interested in my other crystallography articles. Here is this list, in recommended reading order:

[Introduction to Bravais Lattices](#)

[What is the Difference Between “Crystal Structure” and “Bravais Lattice”](#)

[Atomic Packing Factor](#)

[How to Read Miller Indices](#)

[How to Read Hexagonal Miller-Bravais Indices](#)

[Close-Packed Crystals and Stacking Order](#)

[Interstitial Sites](#)

[Primitive Cells](#)

[How to Read Crystallography Notation](#)

[What are Point Groups](#)

[List of Point Groups](#)

[What are Space Groups](#)

[List of Space Groups](#)

[The 7 Crystal Systems](#)

If you are interested in more details about any specific crystal structure, I have written individual articles about simple crystal structures which correspond to each of the 14 Bravais lattices:

1. [Simple Cubic](#)

2. [Face-Centered Cubic](#)

2a. [Diamond Cubic](#)

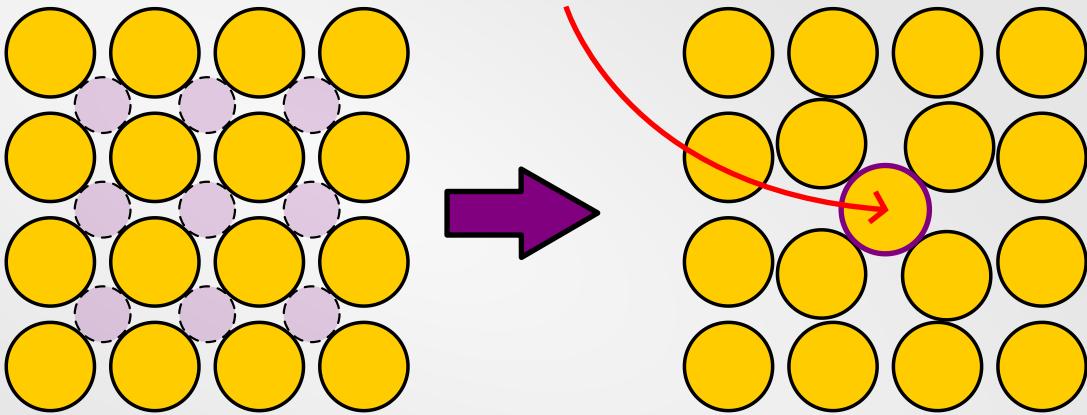
3. [Body-Centered Cubic](#)
4. [Simple Hexagonal](#)
  - 4a. [Hexagonal Close-Packed](#)
  - 4b. [Double Hexagonal Close-Packed \(La-type\)](#)
5. [Rhombohedral](#)
- 5a. [Rhombohedral Close-Packed \(Sm-type\)](#)
6. [Simple Tetragonal](#)
7. [Body-Centered Tetragonal](#)
  - 7a. [Diamond Tetragonal \(White Tin\)](#)
8. [Simple Orthorhombic](#)
9. [Base-Centered Orthorhombic](#)
10. [Face-Centered Orthorhombic](#)
11. [Body-Centered Orthorhombic](#)
12. [Simple Monoclinic](#)
13. [Base-Centered Monoclinic](#)
14. [Triclinic](#)

## Related Questions

### What are self-interstitials?

Self-interstitials are when an atom fits into its own interstitial site. This will be more common with larger interstitial sites (such as simple cubic's cubic interstitial site, or FCC's octahedral interstitial site).

# Self-Interstitial



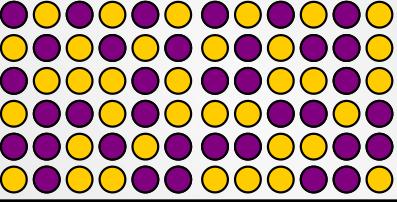
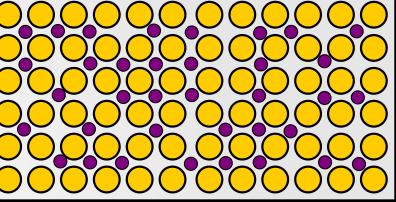
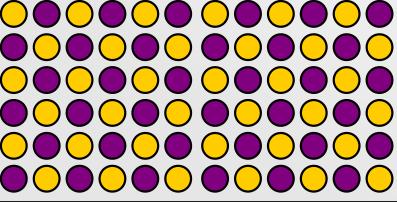
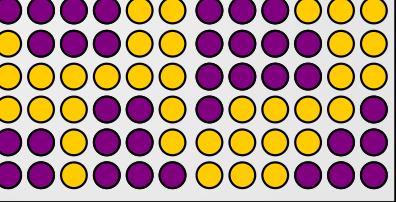
Interstitial sites  
between atoms

An atom of the same type squeezes into the interstitial space.

The atom is too large and distorts the surrounding atoms.

## What is interstitial solid solution?

Alloys can be solid solutions, which means that one type of atom is dissolved in a metal. You probably think of dissolution in a liquid, like salt in water, but this process happens in solids as well. The 2 types of solid solution are “interstitial” and “substitutional.”

<b>Substitutional Alloy</b> (solid solution) ● and ● like each other equally. They can randomly replace each other. 	<b>Interstitial Alloy</b> (solid solution) ● and ● like each other equally. Small atoms randomly squeeze between big atoms. 
<b>Intermetallic Compound</b> ● and ● like each other more than themselves They must be arranged in a specific order to maximize contact. 	<b>Two-Phase Alloy</b> ● and ● like each other less than themselves They stay in distinct phases to minimize contact 

In a substitutional solid solution, the dissolved atom *replaces* the main atom in the crystal structure. In an interstitial solid solution, the dissolved atom sits in an interstitial site among the main atoms in the crystal structure.

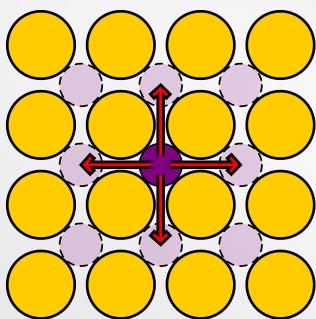
If atoms are about the same size, they will tend to form a substitutional solid solution. If the impurity atom is much smaller than the host atom, it will form an interstitial solid solution.

### What is interstitial diffusion?

Diffusion is when atoms move around by random vibration. For an atom to travel through a metal, it needs to move to an empty space. If the atom is the same size as most of the atoms, these empty spaces are *vacancies*. However, each interstitial site is also an empty space, as long as the atom can fit into it.

Interstitial diffusion is when a small atom—which can fit into the interstitial sites of another atom—is able to rapidly move through the crystal lattice of a larger atom. Interstitial diffusion is much faster than vacancy diffusion, because most materials have many more empty interstitial sites than vacancies. Small atoms such as hydrogen, carbon, nitrogen, and oxygen are most likely to experience interstitial diffusion in metals.

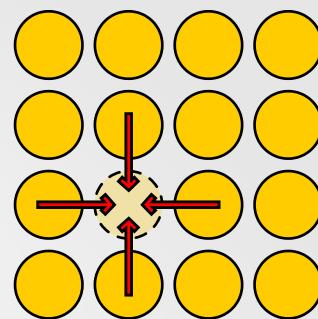
## Interstitial vs Vacancy Diffusion



**Interstitial Diffusion**

One interstitial atom can move to many empty interstitial sites

Interstitial atoms are surrounded by empty space so they usually diffuse **much faster** than host atoms.



**Vacancy Diffusion**

Many host atoms can move to one empty vacancy

**Brandon**

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## Recommended Posts

### **What Are Bravais Lattices? (Definition, Types, Examples)**

Bravais lattices are the basic lattice arrangements. All other lattices can simplify into one of the Bravais lattices. Bravais lattices move a specific basis by translation so that it lines up to an...

[CONTINUE READING](#)

# **What Is the Difference Between FCC and BCC? (Crystal Structure, Properties, Interstitial Sites, and Examples)**

The most direct difference between FCC and BCC crystals is in the atomic arrangements. The face-centered cubic structure has an atom at all 8 corner positions, and at the center of all 6 faces. The...

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