



# 4. A Healthy Relationship: The Structure-Property Relationship



## LEARNING GOALS

### Learning Objectives

1. Generalize the relative positions on a logarithmic plot of strength versus density and Young's modulus versus density of several metals, ceramics, and polymers
2. Identify the region on a plot of Young's modulus versus density where we would like to develop new materials for many applications such as aerospace
3. OPTIONAL: Demonstrate, given the derivation, how the Materials Performance Index for a light stiff beam is determined to be:  
$$\frac{E^{1/2}}{\rho}$$
4. Define the dimensions of density, and name commonly used units
5. Show how knowledge of a material's crystal structure can be used to calculate the theoretical density
6. Compare and contrast long-range and short range order and no order
7. Recall several examples of ordered solids in each of the three material classes (metals, ceramics, and polymers)
8. Illustrate how the macroscopic features of a crystal may be representative of features of the atomic arrangement
9. Using the face centred cubic crystal structure, illustrate how the theoretical density of a polycrystalline metal can be calculated from knowledge of the crystal structure, atomic radius, and atomic weight
10. Calculate the theoretical density of an FCC metal given the atomic weight, crystal structure and atomic radius
11. Show that the atomic packing factor (APF) for FCC is 0.74



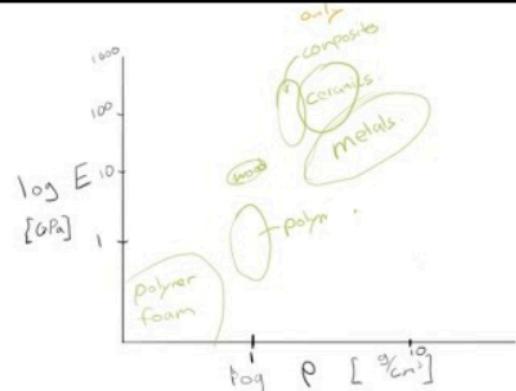
### Lightweight Materials

What do we want from things these days? Okay, very broad question, so I'll answer it myself. Very often we want things to be lighter: thus the title of this section. I should have added a spoiler alert. But why do we want lighter cars, lighter aircraft, lighter sporting goods, etc? Well, there are environmental benefits through decreased fuel costs. That's better for our planet. There's also improved performance



through higher power to weight ratios for vehicles and more rapid responses with sporting goods. Then there's the comfort and ease of use of a lighter product. Can you imagine this: *Introducing the latest iPhone Xls - our heaviest phone yet!* Okay, you're right, if they built it someone would buy it, but I think you get the idea here. Lighter is better <sup>1</sup>①

## In Life, Nothing is Free



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Often it is helpful to consider relationships between material properties. For instance, how does Young's modulus change with changes in density?

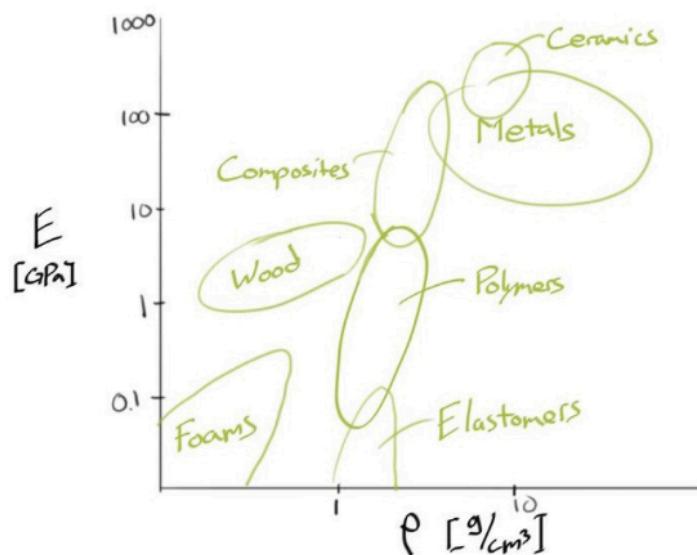


Figure 1: A plot of Young's modulus versus density on logarithmic axes.

Figure 1 illustrates how there is generally an increase in density as we move to higher Young's modulus. Incidentally, these plots of material properties illustrating groups of materials in envelopes, or roughly oval-ish regions, were first introduced by Mike Ashby from Cambridge University. Ashby is a godfather

of materials science. Looking at Figure 1 you'll also likely notice that the upper left region of the plot, corresponding to light weight stiff materials is empty. This is an important area of current research. Composite materials like carbon fibre or even fibreglass help us move slightly into this region. Research into new materials like carbon nanotubes offer some hope that we may eventually populate this region.



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## Example: Lightweight Ladders, Racquets, and Rotors

What do ladders, tennis racquets and helicopter rotors have in common? They are all loaded in bending at least some of the time. If we consider only the rungs of the ladder, then the loading is even more predominantly in bending. This is another way of saying that these components are beams. Alright, the rotor is arguable more of a plate, but it is loaded in bending. I thought it made for a catchy title. Thanks for going along with my shenanigans. Let's dive into this in more detail. The beautiful materials selection process that Mike Ashby pioneered involves starting with an *objective function*: something that we want to maximize or minimize. In all three of these examples, we want to minimize mass, so the objective equation is:

$$m = AL\rho$$

where  $A$  is the cross-sectional area of the ladder rung, helicopter rotor, or the handle of a tennis racquet. Next, we define a constraint for our design. In this case, we are going to consider *elastic* bending, meaning that we impose a maximum deflection constraint. That is, if the rung, racquet, or rotor, bends more than a certain amount, even without plastic deformation or fracture, it fails to meet our design requirements. The deflection of a beam takes the form of this equation:

$$\delta = \frac{FL^3}{CEA^2}$$

where  $F$  is the force applied,  $L$  is the span-length of the beam,  $C$  is a constant,  $E$  is the Young's modulus.

Since the length  $L$  of our component is prescribed by the design, we cannot change the length. However, we can change the cross sectional area of the beam and still achieve our design objective of spanning a distance. With this in mind, we call the cross-sectional area  $A$  our *free-variable* and rearrange our constraint so the area is expressed in terms of all the other variables

$$A = \left( \frac{FL^3}{CE\delta} \right)^{\frac{1}{2}}$$

Now we substitute this free variable equation back into our objective function

$$m = \left( \frac{FL^3}{CE\delta} \right)^{\frac{1}{2}} L\rho$$

Now, considering only the *material properties* we see that in order to minimize the mass, we must minimize  $\frac{\rho}{E^{\frac{1}{2}}}$  or, by convention in the form to maximize we define the reciprocal of this as our *Materials Performance Index* or

$$MPI = \frac{E^{\frac{1}{2}}}{\rho}$$

Which we can plot on our  $E$  versus  $\rho$  chart by taking the log of both sides and rearranging

$$\log E = 2 \log \rho + 2 \log MPI$$

which gives us a line with a slope of 2, which we can move higher to yield higher values of the MPI and identify materials better suited to use as a light stiff beam. Sketch a line with a slope of 2 on Figure 1 and move the line towards the top left. The last materials you'll be left with are composites and ceramics. We eliminate ceramics since they are susceptible to catastrophic brittle fracture. This leaves the composites and the best among them generally being carbon fibre reinforced polymer, or CFRP. A similar analysis for a light stiff plate, in which the thickness is the free variable, with the horizontal area of the rotor fixed yields an  $MPI$  of  $\frac{E^{\frac{1}{2}}}{\rho}$ . Plotting this line and moving it up gives a very interesting result: wood performs very well as a stiff light plate. Of course, this is not surprising considering that the propellers on early aircraft were made from wood.

## Mass Density (Plain Old Density)

So, by now, we all agree that low density is often a good quality for materials. I'd like to dive into density in a little more detail now and use it as a springboard to dive into the fascinating microstructure of solids. When we say density most often we mean mass density rather than, say, charge density, or bond density. Density is a measure of mass per unit volume and the base SI units would be kg

Density. Density is a measure of mass per unit volume and the base SI units would be  $\text{m}^3$

although most often we'll be a little rebellious, throw cation to the wind and enjoy the easy and familiar convenience of the non-SI  $\frac{\text{g}}{\text{cm}^3}$ . Of course, the  $\frac{\text{g}}{\text{m}^3}$  could be used, but this is highly unconventional and is not used in practice. How do I connect density then to the structure of solids? Brace yourself.



## EXERCISE YOUR KNOWLEDGE



Q4.4.1  
Review

Mark as: None ▾

Which of the following is NOT a conventional unit for density?

Select an answer and submit. For keyboard navigation, use the up/down arrow keys to select an answer.

a  $\frac{\text{g}}{\text{m}^3}$

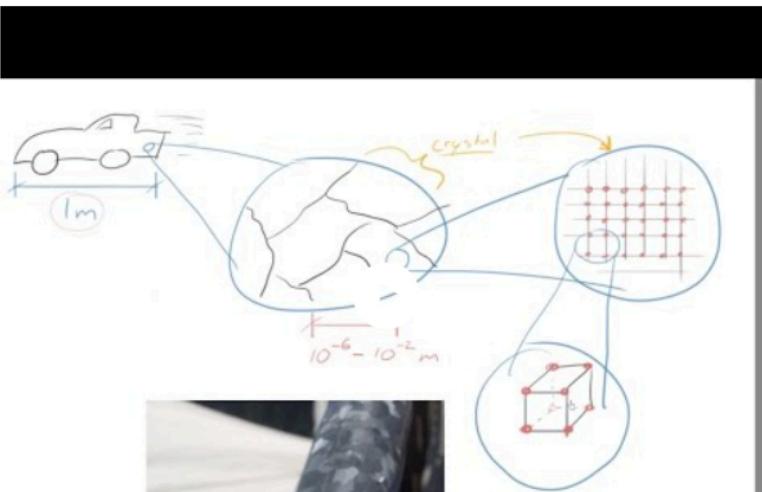
b  $\frac{\text{g}}{\text{cm}^3}$

c  $\frac{\text{kg}}{\text{m}^3}$

d  $\frac{\text{g}}{\text{cc}}$

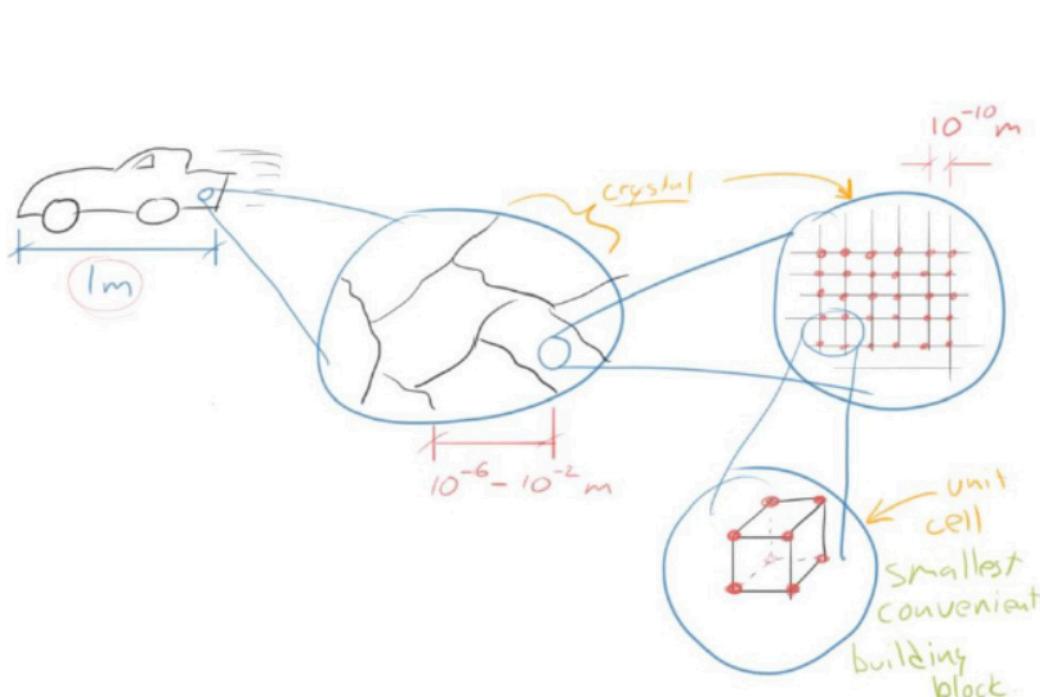


## Ordered Solids. Who Ordered Solids?



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What? You don't get the title? You know, as if someone went to a restaurant and ordered solid food. I know, jokes are so much better when they need to be explained. Really though, so much of the solid matter that we interact with every day is beautifully arranged at, and close to, the atomic scale. Just about any metal around you, with a few exceptions<sup>2</sup>① is *polycrystalline* meaning it is made of crystals, typically around the micron scale.



**Figure 2:** The side panels of a car, such as this beautiful little sporty coupe, are typically steel and the steel is made of tiny little crystals of regularly arranged iron atoms.

Figure 2 attempts to give a sense for the approximate order of magnitude of the linear dimensions of these crystals. Each of these crystals is made of a massive number of atoms all positioned in regular repeating positions, spaced roughly at the *atomic scale* which is  $10^{-10}$  m or the Angstrom Å. In the field of materials science or solid state chemistry, these crystals that make up polycrystalline materials are called *grains*.





**Figure 3:** A galvanized steel handrail, such as this one is a steel structure that has been coated in zinc to protect the steel from corrosion. Frequently these zinc grains are quite large and can be seen with your naked eyes

A common place that you may have seen grains, perhaps without realizing it, is on galvanized steel lamp posts, street signs, railings, and such. Figure 3 shows such a hand rail with the zinc grains beautifully exposed through the action of thousands of sweaty hands slowly polishing the surface and preferentially etching away atoms that exist at the boundaries between grains: the so-called *grain boundaries*. Figure 2 also shows us the so-called *unit cell* or the smallest convenient repeating unit that we can use to accurately represent the overall crystal. Even though a crystal or grain of metal may contain say, to ballpark, roughly  $10^{19}$ – $10^{20}$  atoms, we can simplify this massive repeating structure down to a single convenient unit cell, or building block that accurately describes the crystal. This type of highly ordered repeating structure that extends well beyond the scale of the atom, or even tens or thousands of atoms is known as *long range order*. In some materials we only have knowledge of the positions of nearest neighbour atoms, but beyond that there is no long range order. Surprise, surprise, such materials are said to have only *short range order*. When it comes to long range order, nature is merciful and it turns out that many elements form crystals having cubic symmetry. See, I told you I'd get from density to crystal structure.



## EXERCISE YOUR KNOWLEDGE



Q4.6.1  
Review

Mark as: None ▾

Which of the following is closest to the atomic scale?

Select an answer and submit. For keyboard navigation, use the up/down arrow keys to select an answer.

a  $10 \times 10^{-14}\text{m}$

b  $10 \times 10^{-6}\text{m}$

c  $10 \times 10^{-10}\text{m}$

d

$$10 \times 10^{-23} \text{m}$$



Q4.7.1  
Review

Mark as: None ▾

Which of the following is not an example of a highly ordered solid?

Select an answer and submit. For keyboard navigation, use the up/down arrow keys to select an answer.

a A glass window

b A brass door nob

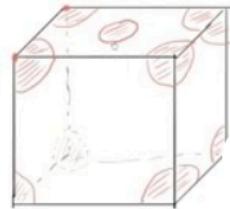
c A diamond

d A steel nail



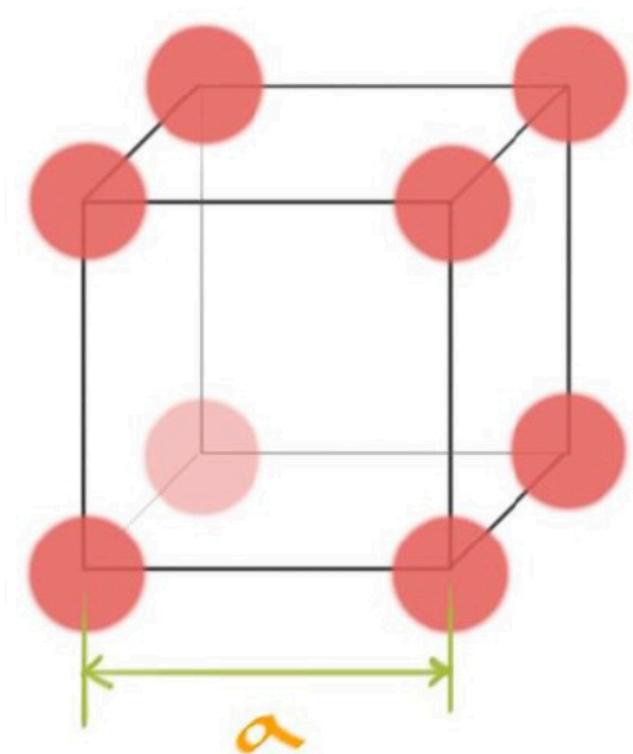
## Face-centred Cubic or FCC

Ex Face-centred cubic (FCC) many metals  
ex Al.



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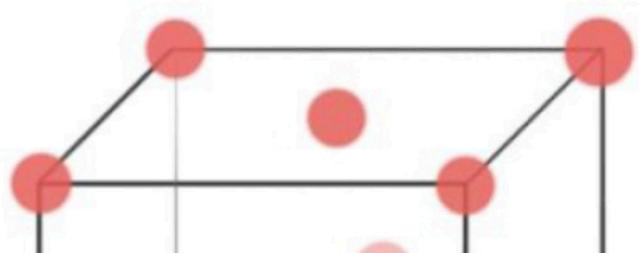
The first crystal structure that we'll study is *face centred cubic* or *FCC*. The name is fairly descriptive: first of all, it is cubic, meaning that we will position the centre of an atom at each of the corners of a cube, as shown in Figure 4.

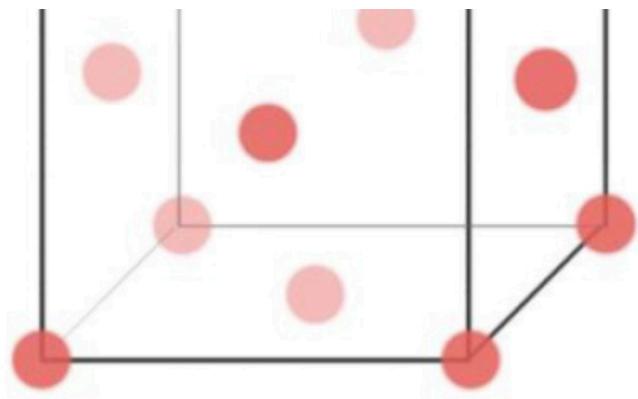


**Figure 4:** The simple cubic unit cell, showing an atom centred at each of the eight corners of a cube. The lighter red dots are the atoms located on the hidden parts of the cube. The cube edge length is known as the lattice parameter and is denoted with the letter  $a$ .

This crystal structure is known as *simple cubic* but is not particularly useful to study since it is very rare with only one element forming this structure. It is worthwhile noting at this point that we only need to define one dimension for our unit cell, since it is a cube. The cube edge length is known as the *lattice parameter*  $a$ .

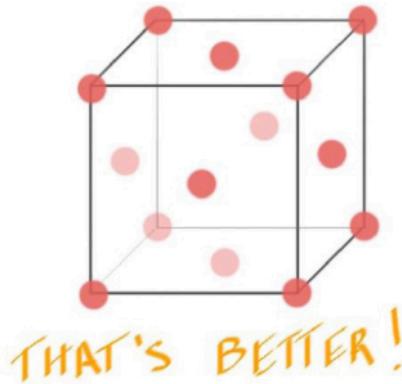
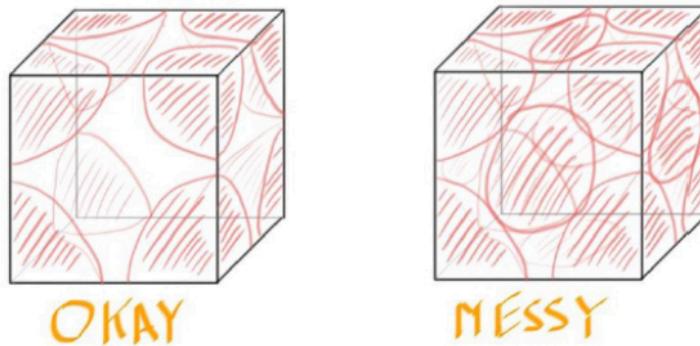
Now, on to the other atoms in the FCC unit cell: the *face centred* atoms. As the name suggests, these atoms are centred on each of the six faces of the cube, as shown in Figure 5.





**Figure 5:** The FCC unit cell, showing an atom centred at each of the eight corners of a cube as well as one atom centred at the very centre of each of the six cube faces. The lighter red dots are the atoms located on the hidden parts of the cube.

At this point you may well be wondering why I've drawn the atoms as little red dots and why I've apparently been so cavalier about the size of these dots. I mean, have I no respect at all for science? How can I change the size of atoms on a whim? Well, these are good questions. First, I do respect science. Science is the truth<sup>①</sup>.

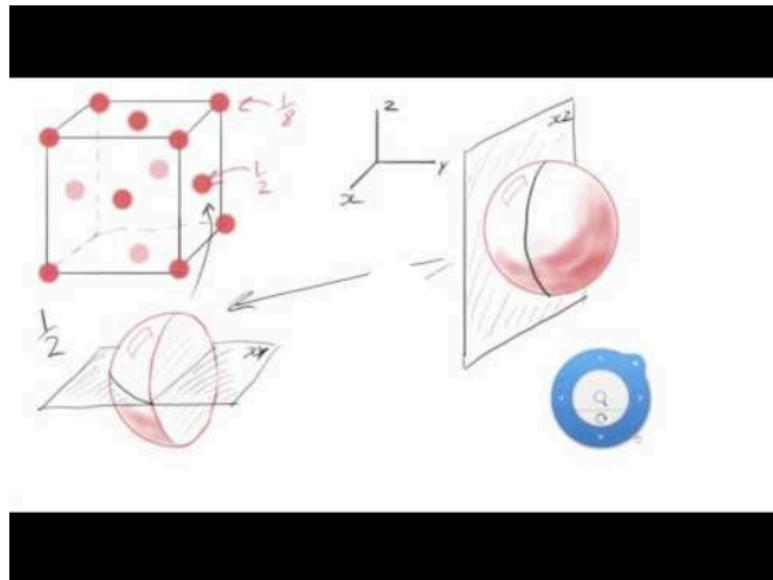


**Figure 6:** This is me trying to show you how messy the full hard sphere model can get. It's hard to draw and hard to look at. In the top left, I've drawn the corner atoms only from the FCC crystal structure. Then, to the right I've drawn in the face centred atoms. Wow! That got messy real quick. Let's stick to the reduced sphere depiction of the hard sphere model.

Regarding the second point, the size of the atoms, well, our crystal structures are based on a model

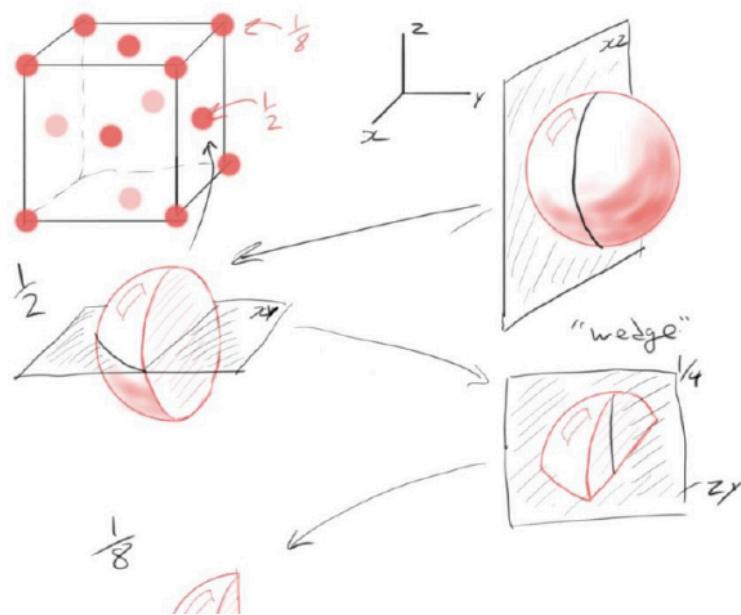
known as the *hard sphere model* that treats the atoms in ordered solids as hard spheres that make contact with their nearest neighbour atoms at distances defined by the atomic radii, taken to be fixed. That is, we treat atoms, well, *hard sphere*. We are only concerned with the fractions of these spheres that reside within our unit cell, but it quickly becomes tedious to draw out the full hard sphere depiction, so we often take a shortcut and draw the atoms as simple dots, and call it the *reduced sphere model*.

The nuclei stay in the same positions, but we just make the atoms smaller to make it easier to draw and much easier to see, as I've tried to illustrate in Figure 6.



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Now, there is still the matter of what fraction of atom is actually inside the cube at each position. I've attempted to draw a sphere being sliced up in Figure 7.





**Figure 7:** A sphere being sliced in one plane to yield two half spheres, two planes to yield four quarter spheres or "wedges", and three planes to yield eight eighths, as you would find in each of the corners of the cube.

The FCC unit cell doesn't contain any of the quarter spheres or *wedges*, but don't worry, we'll see those positions when we cover the *Rock Salt* crystal structure later. The eight atoms that result from a sphere being sliced in three orthogonal planes are found in the eight corners, while the half atoms are located at the face centred positions. So, in total, there is  $8 \cdot \frac{1}{8} = 1$  atom contributed from the corners, plus  $6 \cdot \frac{1}{2} = 3$  atoms from the faces for a total of 4 atoms in the FCC unit cell  $n_{FCC} = 4$  (1)



## And Back to Density Again

Let's put our new knowledge to the test. Something fairly obvious and relatively straightforward that we could calculate with knowledge of crystal structure would be the density. We already established the units of density, so let's think about how we could calculate that using a basis of a single unit cell. Since density is mass per unit volume the numerator must express the mass of all of the atoms in the unit cell

$$\text{Mass}_{\text{Atoms in Unit Cell}} = \text{Number}_{\text{Atoms in Unit Cell}} \cdot \frac{\text{Molar Mass of Atom}}{\text{Avagadro's Number}} \quad (2)$$

or

$$m = n \cdot \frac{A}{N_A} \quad (3)$$

And the denominator would simply be the volume of the unit cell  $V_C$ , meaning that the *Theoretical Density* of a crystalline solid is

$$\rho = \frac{nA}{V_C N_A} \quad (4)$$



where  $\rho$  is the Greek letter *rho*, used for density,  $n$  is the number of atoms within the unit cell,  $A$  is the molar mass of the element,  $V_C$  is the volume of the unit cell, and  $N_A$  is Avagadro's Number.

$$V_C = a^3$$

$$\rho = \frac{nA}{V_C N_A} \quad \left| \begin{array}{l} n=4 \\ A=26.982 \text{ g/mol} \\ N_A=6.023 \cdot 10^{23} \text{ mol}^{-1} \end{array} \right.$$

$a^2 + a^2 = (4R)^2$   
 $2a^2 = 16R^2$

$$= (2\sqrt{2}R)$$

$$\frac{\sqrt{3}}{2}$$

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



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## EXERCISE YOUR KNOWLEDGE



Q4.10.1

Review

Mark as: [None ▾](#)

Assuming an atomic radius for aluminum of 184 pm, an atomic mass of 26.982  $\frac{\text{g}}{\text{mol}}$  and the FCC crystal structure, calculate the theoretical density of aluminum in  $\frac{\text{g}}{\text{cm}^3}$ . Express your final answer with 2 significant figures and do not include units in your response.

Type your numeric answer and submit



## The Atomic Packing Factor

A concept closely related to the mass density is the *Atomic Packing Factor* APF, as it is commonly known, or the *Volume Packing Fraction* as I sometimes prefer to call it. Since APF is the name commonly used, I'll stick with that here. This is a measure of the fraction of a volume that is occupied by atoms arranged in a particular crystal structure

$$\text{APF} = \frac{\text{Volume}_{\text{Spheres}}}{\text{Volume}_{\text{Unit Cell}}} \quad (5)$$

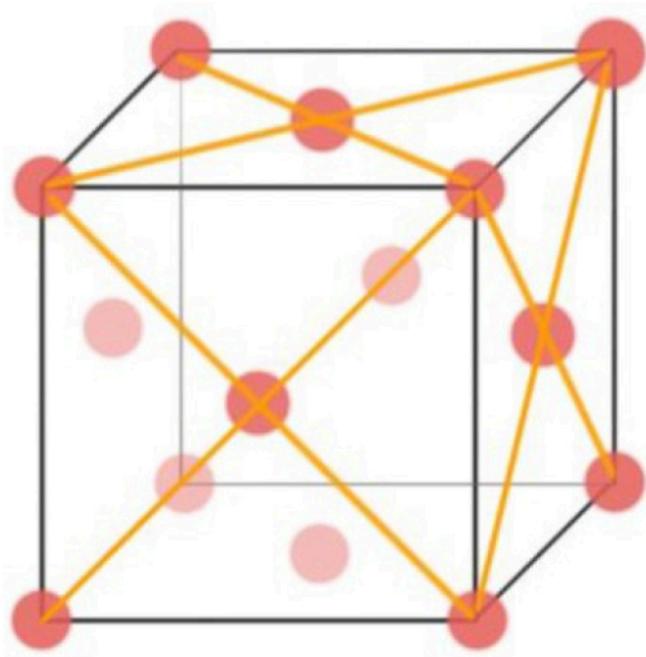
or, since the unit cell is a cube whose volume is  $a^3$

$$\text{APF} = \frac{n \frac{4}{3} \pi R^3}{a^3} \quad (6)$$

and, specifically for FCC

$$APF = \frac{\frac{4}{3}\pi R^3}{a^3} \quad (7)$$

But wait! There is a pesky  $R^3$  in the numerator and an  $a^3$  in the denominator. Can't we do better to clean this up? Well, we can in fact.



**Figure 8:** The direction of contact between atoms in the FCC unit cell is along the cube face diagonals, as illustrated by the orange lines.

You see, what I didn't yet tell you is how the atoms in the FCC unit cell make contact with one another.

The atoms in the FCC unit cell touch along the *face diagonals* as shown in Figure 8. Since the edge length is  $a$ , we can use the Pythagorean Theorem to calculate the lattice parameter in terms of the

$$\begin{aligned} a^2 + a^2 &= (4R)^2 \\ 2a^2 &= 16R^2 \end{aligned} \quad (8)$$

$$a_{FCC} = 2\sqrt{2}R \quad (9)$$

Which we can substitute back into our APF equation to give

$$APF = \frac{\frac{4}{3}\pi R^3}{(2\sqrt{2}R)^3} \quad (10)$$

$$APF_{FCC} = 0.74 \quad (11)$$

It turns out that this APF is actually the highest possible for packing with a single diameter of sphere. The interesting feature of this result is that it is independent of atomic radius, meaning that whether you have spheres the size of yoga balls or spheres only a micron in diameter, the maximum fraction of a volume that can possibly be filled with spheres is 74%.



Q4.12.1  
Review

Mark as: None ▾

A bean bag chair is filled with tiny styrofoam spheres 1.2 mm in diameter. All of the spheres have the same diameter. If the bean bag chair has a volume of 195 L, what is the maximum volume of styrofoam that would be needed to fill this chair? Express your final answer in L to three significant figures and do not include units in your final answer.

Type your numeric answer and submit

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