- *Structural defects vs. ductility*

  One finds that within the class of metals, in pure metals deviations from structural perfection have a great deal of influence on ductility, and on mechanical properties in general.

  In addition, alloys behave rather differently in comparison to their corresponding pure metals. By and large, alloys are stronger but less ductile than the pure metals. Think of an alloy as a base metal with other metallic impurities, i.e. a base metal with compositional defects.

We will encounter these and other structure-property connections over and over again, and in due time a fairly complete picture of them will emerge.

3.2 Crystals and Unit Cells

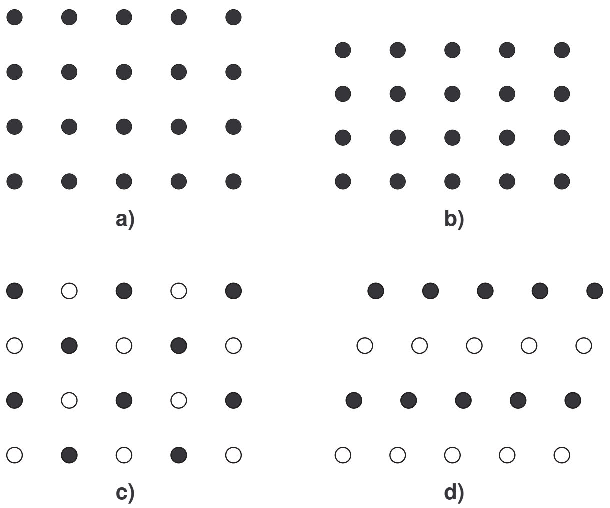

Figure 3.1: Examples of possible two-dimensional (2D) crystals

As we have indicated, many materials found in nature, or engineered by people, are in crystalline form. By **crystalline**, or being **crystals**, we mean that the atom positions in these materials form a regular array, so that you can move from a particular atom in various directions to another identical atom with the exact same surroundings. In other words: The local structure around an atom repeats itself over many thousands of atomic distance. Such a repeating arrangement of atoms in a crystal is also said to exhibit **long-range order**.

Fig. 3.1 gives a few examples in two dimensions, but of course in a real material you should visualize the regularity, or repeating property, as occurring in the third dimension as well. You can see readily 2D crystals in this figure, i.e. structures that repeat themselves. Clearly, the regularity could extend over a large distance, including many atoms. You could describe the regularity of the structure of Fig. 3.1a as square, Fig. 3.1b as rectangular but not square, Fig. 3.1c as square but with two kinds of atoms, and Fig. 3.1d as not rectangular with two kinds of atoms.

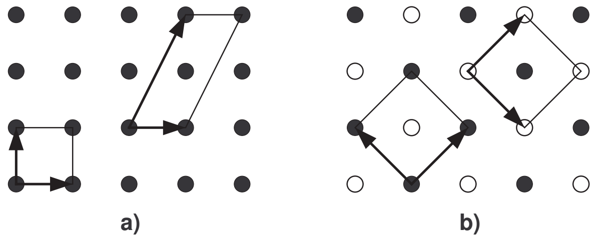

Figure 3.2: Examples of possible unit cells in 2D crystals

Now we need to become a little more systematic about dealing with the regularity of crystals. To this end, we introduce the notion of a **unit cell** (Fig. 3.2). This figure shows two of the structures from Fig. 3.1 before, each with two of many possible unit cells. The only requirement on a unit cell is that it allows us to generate the entire crystal. The unit cells shown obviously do.

Each of the unit cells also has two arrows, indicating what is called the **unit vectors** of the unit cell. When we want to describe the entire crystal, the rule is that when we move a unit cell, with its atoms, by a multiple of either of the unit vectors, we get to a position which is identical to the original one. Note that this means that the small square in Fig. 3.1a is a unit cell, but the same-sized small square in Fig. 3.1b is not. When you move the unit cell according to the rule above, black atoms have to end up on black atoms, and white atoms on white atoms.

Sometimes it is also of interest to speak of the **lattice** underlying a crystal structure. Think of the lattice as a geometrical abstraction, the grid on which the atoms are laid out. For example, we would say that the structures in Fig. 3.1a and Fig. 3.1b have the same type of square lattice, but the two lattices are populated by atoms in a different way. You will have ample opportunity to practice using these concepts when we talk about three-dimensional structures.

3.3 Close-Packing of Atoms

We noted in Chapter 2 that metallic bonding can be envisioned as the result of metal atom cores being immersed in a sea of highly mobile electrons. Furthermore, a key feature of this type of bonding is that it is non-directional. That is, the interaction between two atoms is independent of the direction in which they approach each other. This simple principle, together with some straightforward refinements, will allow us to account for essentially all crystal structures observed in metals.

Imagine that we build a metal crystal out of spheres stuck together. The spheres have an attractive interaction when they are close enough to each other, but they also have a given diameter that defines how close two spheres can come. Think of the spheres as billiard balls with mutual attraction.

The rule is that we ***build the configuration with the lowest possible energy***. This means that we will try for each sphere to touch as many other spheres as possible.

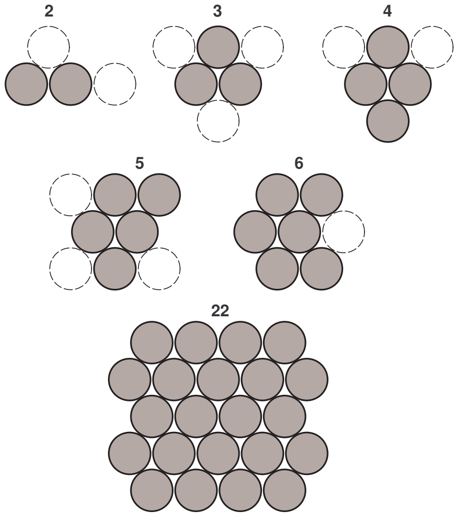

Figure 3.3: Atom-by-atom formation of a metal crystal. The numbers label clusters by their original number of atoms. With clusters 3, 4, and 5, the dashed circles indicate some of the equivalent positions for adding the next atom. For cluster 2, the two positions are not equivalent, and for cluster 6, the position shown is the best one.

Now let us put together a crystal, adding one atom at a time, using our engineering common sense. The first few steps are illustrated in Fig. 3.3. You have noted, of course, that the growth of this crystal was forced to occur in two dimensions. Beginning with the cluster labeled 3, there are even better positions if we allow for the third dimension to be used:

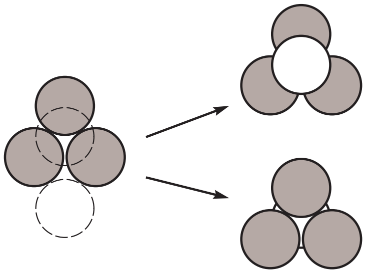

Figure 3.4: The two best positions for atom 4, on top or below the triangle of the first three atoms. In each case, the 4 atoms form a tetrahedron, and each atom touches the 3 other atoms.

It should be evident how we proceed to build a large crystals: Take layers of hexagonally arranged atoms, such as cluster 22 in Fig. 3.3, and put them on top of each other. The next figure shows two such layers, and the light gray one goes either on top or at the bottom of the dark gray one.

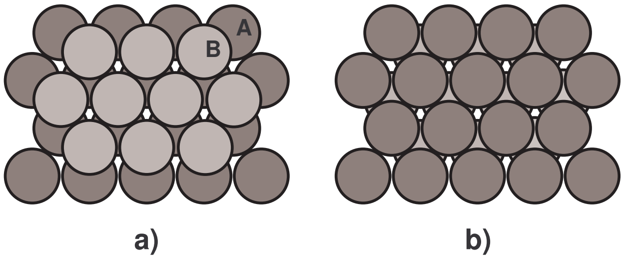

Figure 3.5: Two hexagonal atom layers put on top of each other. a) Second layer on top of first; b) Second layer at bottom of first layer.

The really interesting action happens with the third layer. Look carefully at the two graphics in Fig. 3.5, and you will realize that *once we have two layers, there are two different ways for putting down the third layer*! This is easiest to see when you focus on the light gray layer B in Fig. 3.5a: There are two types of sites for the third layer, depending on whether the spaces in-between the light gray atoms are open underneath or occupied by dark gray atoms.

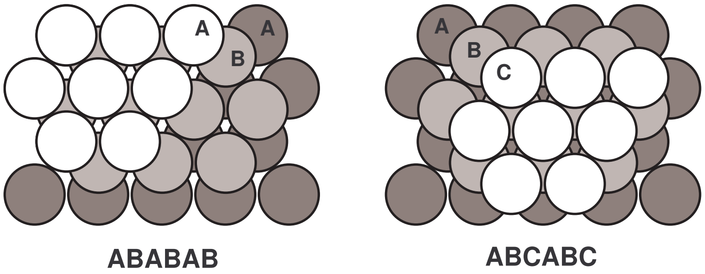

Figure 3.6: The two possible sequences for stacking three hexagonal layers. The layers marked A are exactly on top of each other, i.e. exactly in the same horizontal position.

Note that with the ABABAB stacking, vertical "channels" are left open between the atoms, but with the ABCABC stacking there are no open "channels".

Both these stacking sequences achieve what we will refer to as **close-packing**, and we will call the structures **close-packed**. The term should be clear: Hexagonal layers is how to pack atoms as closely as possible in a plane, and there are two ways to stack hexagonal planes. The resulting two close-packed structures are so important in materials science that they have special names:

- ***ABABAB sequence*** ⇔ ***hexagonal close-packed structure***
- ***ABCABC sequence*** ⇔ ***cubic close-packed structure***

The first name is evident. We will see below where the second one comes from.

Another way to describe close-packing is to realize that in both structures each atom has the highest possible number of **nearest neighbors**, i.e. each atom touches as many other atoms as possible. In a hexagonal layer each inner atom touches 6 other atoms within that layer (see Fig. 3.3, cluster 22), and then another 3 atoms on top and 3 atoms at the bottom (Fig. 3.5), for a grand *total of 12 nearest neighbors*.

A concise summary of how to pack metal atoms as efficiently as possible would be:

close-packing ⇔ ***maximize number of nearest neighbors***

The structures thus realized turn out to be two of the three most important ones for metal crystals.

3.4 Structure of Metals

3.4.1 Face-centered Cubic Structure

We begin with the structure displayed in the figure below. This structure is called **face-centered cubic** or **FCC** for short. Its feature is a cubic unit cell with additional atoms in the centers of the cube faces.

A few examples of metals having the **FCC** crystal structure are **Al, Cu, Ni, Pd, Ag, Pt** and **Au**.

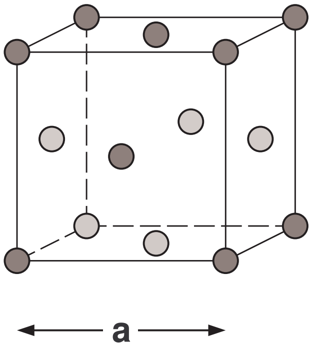

Figure 3.7: Face-centered cubic (FCC) unit cell

Note that all atoms in the cube are of course the same; the ones drawn in dark gray are those you would see if the cube were non-transparent, and the light gray ones are those that would be obscured.

But even more importantly, the atoms in the corners are not in any way different from those in the centers of the cube faces! You can convince yourself easily by looking at four unit cubes combined (Fig. 3.8). The cube with the dark lines is really identical in every way to the four cubes with lighter lines.