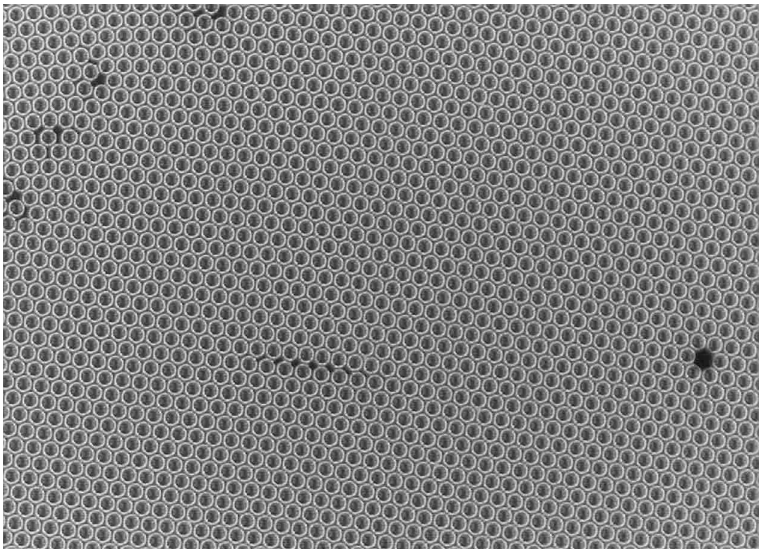
Bubble raft model of a crystal with imperfections



The picture above shows a so-called bubble raft model of a crystal plane with three types of imperfections. (It is an actual layer of soap bubbles.) In the upper right quadrant and elsewhere you can see a perfect hexagonal close-packed layer of bubbles. Near the right edge is a vacancy, a missing bubble. Slightly below the middle is a dislocation; it looks like a small local tear in the hexagonal fabric. Near the upper left hand corner is a grain boundary, a region where two pieces of crystal come together at an angle, i.e. with a slight misorientation.

4 Defects in Solids

In our discussion of the structure of materials we have concentrated so far on crystals and, to a lesser extent, on amorphous materials. With respect to crystals, the tacit assumption was that we were dealing with a **single crystal**, i.e. with a piece of material in which the unit cell repeats itself throughout. It is possible to grow single crystals of many materials, especially most elements, but only with considerable effort. Single crystals are available commercially, but are rather expensive.

Most engineering materials are not single crystals, notable exceptions being silicon and other semiconductor materials used in integrated solid state devices. The reason is that for these devices only single crystals provide the necessary properties, whereas e.g. with structural engineering materials used for their mechanical stability, single crystals would be useless (there is one notable exception here, too, which we will examine later).

Therefore, it is fair to say that most solid engineering materials are polycrystalline or amorphous (or possibly semi-crystalline in the case of polymers). We define a material as **polycrystalline** if it consists of a huge number of tiny crystals of somewhat variable size, oriented fairly randomly relative to each other. (Typical sizes of these little crystals, also referred to as **grains**, might range from 100 nm to 10 μm). It follows that engineering materials are not perfectly ordered, at least not over large distances, but contain various kinds of imperfections, or defects (We will use these two words interchangeably). The study of these defects will be the topic of the present chapter.

4.1 Overview of Crystal Imperfections

The picture at the beginning of this chapter uses a bubble raft model to show three examples of crystal imperfections: a vacancy (i.e. a missing atom) at the right edge, a so-called dislocation a little below the middle of the figure, and a grain boundary (the region between two grains) in the upper left corner. All these defects are important in determining various properties of materials, as we shall see in due course.

It is convenient to classify imperfections according to their dimensionality as follows:

1. **Zero-dimensional (0D), or point defects:**

   These defects involve individual lattice sites. The simplest of them is the **vacancy**, i.e. a missing atom (see the figure above). Other point defects are illustrated in Fig. 4.1.

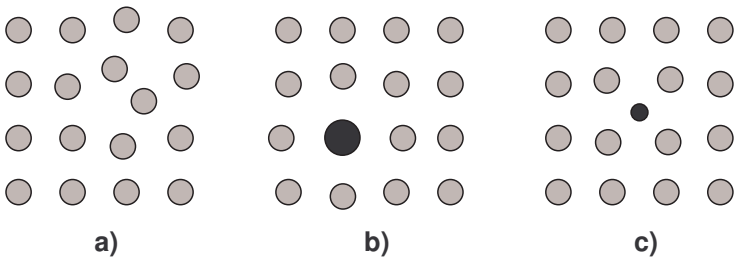


Figure 4.1: Schematic illustration of various types of point defects. a) Self-interstitial; b) substitutional impurity; c) interstitial impurity.

The defect shown in Fig. 4.1a) is called a **self-interstitial**. The word "interstitial" designates the location, namely in-between the regular lattice sites. In a real material, such a defect will also distort the lattice around it because two atoms now have to fit into the space for one. Fig. 4.1b) illustrates a so-called **substitutional** impurity, i.e. an impurity which replaces an original atom at its lattice site. Fig. 4.1c) shows an **interstitial**, i.e an impurity located in-between lattice sites. Both these types of defects generally also result in lattice distortion.

2. **One-dimensional (1D), or line defects:**

   This type of defect is easy to spot in the title figure, but hard to visualize properly. In Fig. 4.2 below I have drawn a magnified schematic view of that defect region, with horizontal rows numbered.

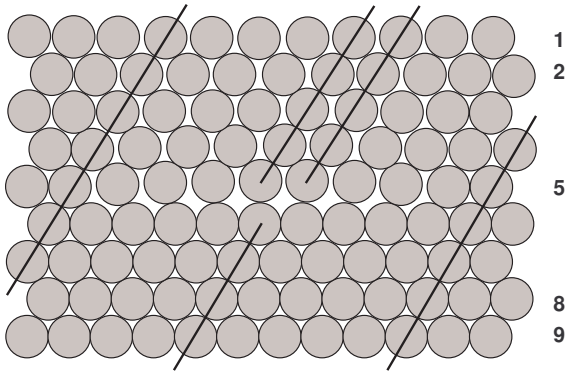


Figure 4.2: Region around the bubble raft dislocation.

The lines on the two sides are meant to align your view along close-packed directions in the hexagonal pattern. If you count atoms in rows

1 and 9, you will realize that row 1 has 11 atoms in it and row 9 has 12. This mismatch shows up clearly in rows 4 and 5, where it appears as if one extra line of atoms in the bottom half has been inserted between two lines of atoms in the top half.

You will note that in row 1 atoms appear to be lined up pretty well again, but you still have 11 atoms fit into the space where 12 atoms are in row 9. So in row 1 the atoms are separated a little farther than they would be in a true equilibrium configuration. It is as if a force has pulled them apart a little, and by way of reaction they are trying to contract. Another way to describe this situation is that the region around a dislocation is stressed.

3. **Two-dimensional (2D), or area defects:**

   There are two kinds of 2D defects: Grain boundaries (internal surfaces), and the external surfaces of a material.

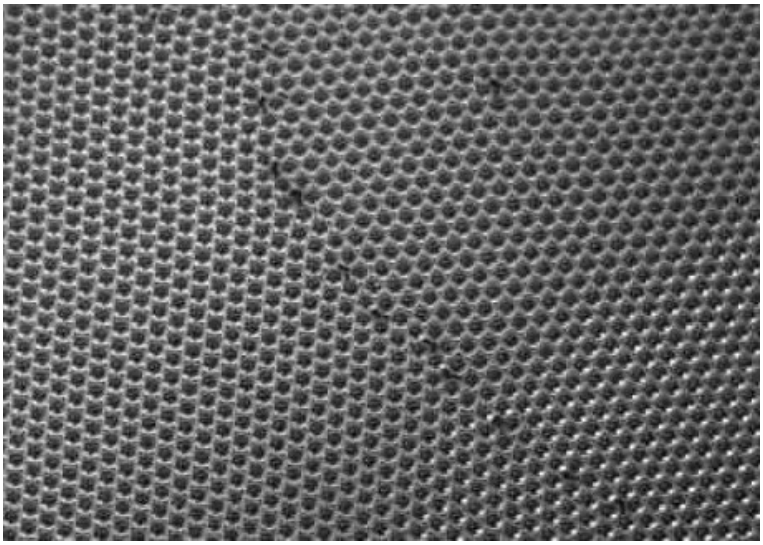


Figure 4.3: Bubble raft model showing a grain boundary between two grains.

We will not discuss external surfaces in any detail in this book. However, grain boundaries will play an important role for us. An example of a grain boundary can be discerned in the upper left corner of the figure at the very beginning of this chapter, but it is not easy to see. Fig. 4.3, which is another bubble raft image, depicts two grains, with their boundary running diagonally across the picture. Note the difference in the alignment of the "atom" rows above and below the grain boundary. (Also note the dislocation in the upper right quadrant).