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Crystalline Silicon Solar Cells

As we already discussed in Chapter 6, most semiconductor materials have a *crystalline lattice* structure. As a starting point for our discussion on crystalline silicon PV technology, we will take a closer look at some properties of the crystal lattice.

12.1 Crystalline silicon

In such a lattice, the atoms are arranged in a certain pattern that repeats itself. The lattice thus has *long-range order* and *symmetry*. However, the pattern is not the same in every direction. In other words, if we make a large cut through the lattice, the various planes you can make do not look the same.

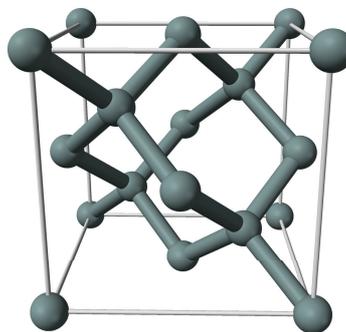


Figure 12.1: A unit cell of a diamond cubic crystal [30].

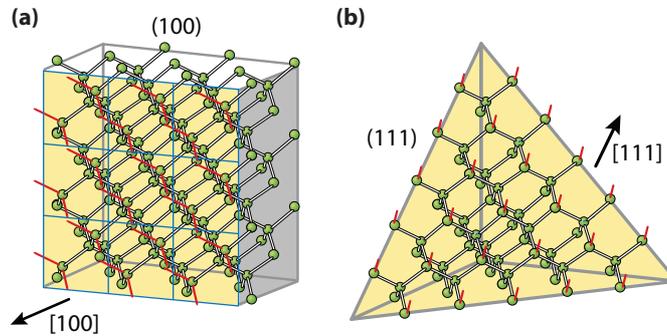


Figure 12.2: The (a) 100 and the (b) 111 surfaces of a silicon crystal.

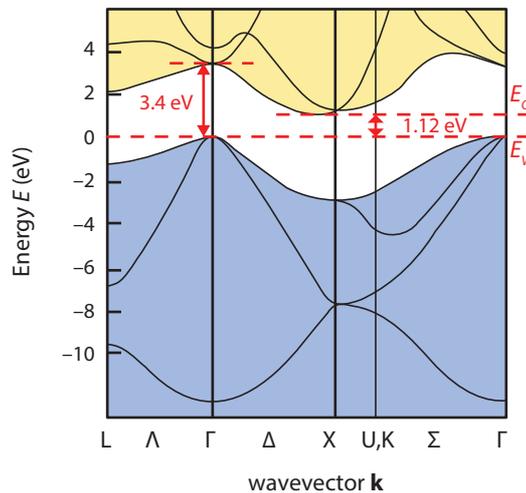


Figure 12.3: The band diagram of crystalline silicon.

Crystalline silicon has a density of 2.3290 g/cm^3 and a *diamond cubic crystal structure* with a lattice constant of 543.07 pm , as illustrated in Fig. 12.1. Figure 12.2 shows two different sections through a crystalline silicon lattice, which originally consisted out of three by three by three unit cells. The first surface shown in Fig. 12.2 (a) is the *100 surface*, whose surface normal is the 100 direction. At a 100 surface, each Si atom has two back bonds and two valence electrons pointing to the front. The second surface, shown in Fig. 12.2 (b), is the *111 surface*. Here, every Si atom has three back bonds and one valence electron pointing towards the plane normal.

To understand the importance of these directions, we look at the *electronic band dispersion diagram* for silicon, shown in Fig. 12.3. On the vertical axis, the energy position of the valence and conduction bands is shown. The horizontal axis shows the crystal momentum, *i.e.* the momentum of the charge carriers. The white area represents the energy levels in the forbidden band gap. The band gap of silicon is determined by the lowest energy point of

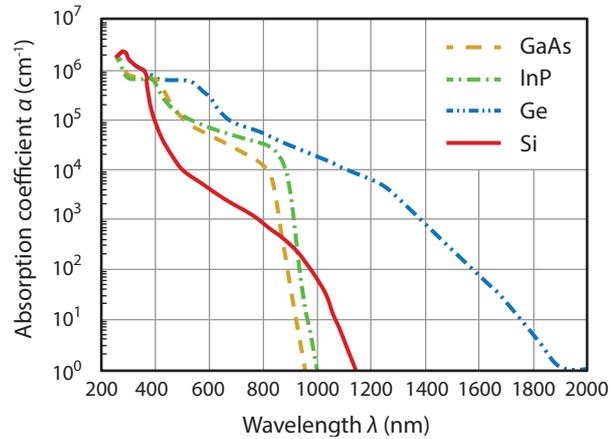


Figure 12.4: Absorption coefficients of different semiconductors.

the conduction band at X , which corresponds to the 100 direction, and the highest energy value of the valence band, at Γ . The *band gap energy* is the difference between those two levels and is equal 1.12 eV, or 1107 nm, when expressed in wavelengths. 1107 nm is in the infrared part of the spectrum of light. This bandgap is an *indirect bandgap*, because the charge carriers must change in energy *and* momentum to be excited from the valence to the conduction band. As we can see, crystalline silicon has a direct transition as well. This transition has an energy of 3.4 eV, which is equivalent to a wavelength of 364 nm, which is in the blue spectral part.

Because of the required change in momentum, for an indirect band gap material it is less likely that a photon with an energy exceeding the bandgap can excite the electron, with respect to a direct bandgap material like gallium arsenide (GaAs) or indium phosphide (InP). Consequently, the absorption coefficient of crystalline silicon is significantly lower than that of direct band gap materials, as we can see in Fig. 12.4. While in the visible part of the spectrum c-Si absorbs less than the GaAs and InP, below 364 nm, it absorbs just as much as GaAs and InP, because there silicon has a direct band to band transition as well. Germanium (Ge), also indicated in the figure, is an indirect bandgap material, just like silicon. The bandgap of Ge is 0.67 eV, which means it already starts to absorb light at wavelengths shorter than 1850 nm. In the visible part of the spectrum, germanium has some direct transitions as well.

Let us now take another look at the design rules for solar cells that we introduced in Section 10.4. First, we look at *spectral utilisation*. The c-Si band gap of 1.12 eV means that in theory we can generate a maximum short circuit current density of 45 mA per square centimetre. Let us now consider the second design rule, *i.e. light management*. First, we look at a wavelength around 800 nm, where c-Si has an absorption coefficient of 1000 cm^{-1} . Using the Lambert-Beer law [Eq. (4.25)], we easily can calculate that for realising an absorption of 90% of the incident light at 800 nm, the required absorption path length is 23 μm . Secondly, we look at 970 nm wavelength, where c-Si has an absorption coefficient of 100 cm^{-1} . Hence, an absorption path length of 230 μm is required to absorb 90% of

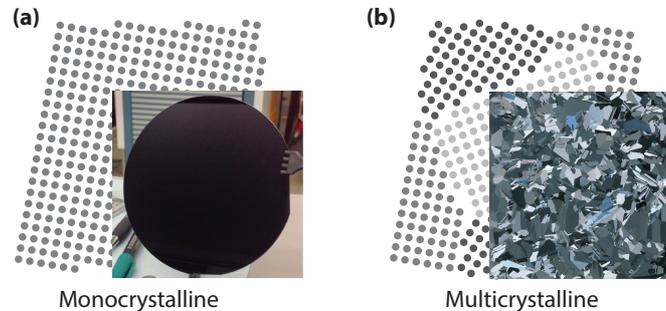


Figure 12.5: Illustrating a (a) monocrystalline and a (b) multicrystalline silicon wafer.

the light. $230\ \mu\text{m}$ is a typical thickness for silicon wafers. This calculation demonstrates that light management techniques become important for crystalline silicon absorber layers above a wavelength of about $900\ \text{nm}$.

Let us now consider the design rule of *bandgap utilisation*, which is determined by the recombination losses. As silicon is an indirect band gap material, only Auger recombination and Shockley-Read-Hall (SRH) recombination will determine the open circuit voltage, while radiative recombination can be neglected. Considering SRH recombination, the recombination rate of the charge carriers is related to the electrons trapped at defect states. When looking at the defect density in the bulk of silicon, we can differentiate between two major types of silicon wafers: *monocrystalline silicon* and *multicrystalline silicon*, which is also called *polycrystalline silicon*.

Monocrystalline silicon, also known as called single-crystalline silicon, is a crystalline solid, in which the crystal lattice is continuous and unbroken without any grain boundaries over the entire bulk, up to the edges. In contrast, polycrystalline silicon, often simply abbreviated with polysilicon, is a material that consists of many small crystalline grains, with random orientations. Between these grains grain boundaries are present. Figure 12.5 shows two pictures of monocrystalline and multicrystalline wafers. While a monocrystalline silicon wafer has one uniform color, in multicrystalline silicon, the various grains are clearly visible for the human eye. At the grain boundaries we find lattice mismatches, resulting in many defects at these boundaries. As a consequence, the charge carrier lifetime for polycrystalline silicon is shorter than for monocrystalline silicon, because of the SRH recombination. The more grain boundaries in the material, the shorter the lifetime of the charge carriers. Hence, the grain size plays an important role in the recombination rate.

Figure 12.6 shows the relationship between the open circuit voltage and the average grain size for various solar cells developed around the world, based on the multicrystalline wafers [46]. The larger the grain size, the longer the charge carrier lifetimes and the larger the band gap utilisation and hence the open circuit voltage will be. On the right hand side of the graph the open circuit voltages of various solar cells, based on monocrystalline wafers, is shown. As monocrystalline silicon has no grain boundary, much larger open circuit voltages can be obtained.

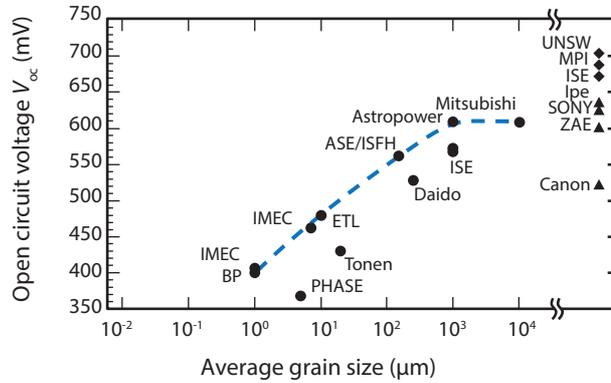


Figure 12.6: The relationship between the open circuit voltage and the average grain size (Reprinted from *Thin Solid Films*, vol. 403-404, R. Bergmann and J. Werner, The future of crystalline silicon films on foreign substrates, Pages 162-169, Copyright (2002), with permission from Elsevier [46].

12.2 Production of silicon wafers

After the initial considerations on designing c-Si solar cells, we now will discuss how monocrystalline and multicrystalline silicon wafers can be produced. In Fig. 12.7 we illustrate the production process of monocrystalline silicon wafers.

The lowest quality of silicon is the so-called metallurgical silicon, which is made from *quartzite*. Quartzite is a rock consisting of almost pure silicon dioxide (SiO_2). For producing silicon the quartzite is molten in a submerged-electrode arc furnace by heating it up to around 1900°C , as illustrated in Fig. 12.7. Then, the molten quartzite is mixed with carbon. As a carbon source, a mixture of coal, coke and wood chips is used. The carbon then starts reacting with the SiO_2 . Since the reactions are rather complex, we will not discuss them in detail here. The overall reaction however can be written as



As a result, carbon monoxide (CO) is formed, which will leave the furnace in the gas phase. In this way, the quartzite is purified from the silicon. After the reactions are finished, the molten silicon that was created during the process is drawn off the furnace and solidified. The purity of metallurgic silicon, shown as a powder in Fig. 12.7, is around 98% to 99%.

About 70% of the worldwide produced metallurgical silicon is used in the aluminium casting industry for make aluminium silicon alloys, which are used in automotive engine blocks. Around 30% are being used for make a variety of chemical products like silicones. Only around 1% of metallurgical silicon is used as a raw product for making electronic grade silicon.

The silicon material with the next higher level of purity is called polysilicon. It is made from a powder of metallurgical silicon in the *Siemens process*. In the process, the metallurgical silicon is brought into a reactor and exposed hydrogen chloride (HCl) at elevated