Chapter 1

Grain Growth

1.1 Introduction

Grain growth is a widely investigated phenomenon in materials science. It influences a large variety of physical and mechanical properties of polycrystalline materials. Grain growth is the result of the collective migration of the grain boundaries and consequence of the necessary topological decay (decrease of the topological and structural elements of the microstructure) that takes place when the average volume of the grains increases. During grain growth both events occur simultaneously, making it a very complex phenomenon. The main driving force for the migration of grain boundaries during grain growth is the area of the boundaries, however, other sources can contribute to the driving force and hence influence grain growth as well. Such sources can be given by a gradient of any intensive thermodynamic variable, for example, temperature, pressure, density of defects, density of energy, etc. In the present chapter, the phenomenology of grain growth will be introduced.

1.2 Grain Boundaries

A polycrystal, as its name indicates, is conformed by many different crystals. Each crystal consists of an ordered three-dimensional arrangement of atoms, which repeats itself, thoroughly the volume of the crystal. These crystals are also known as grains or crystallites. Because each crystal may possess a different orientation, an interface must be formed between two crystals with different orientations when they come into contact. This interface is called grain boundary.

A grain boundary is a very complex structure; its mathematical description requires four parameters in the two-dimensional case and eight parameters in the three-dimensional one. These eight parameters can be discriminated in five macroscopic and three microscopic parameters. The macroscopic parameters are respectively, three Euler angles (φ_1,Φ,φ_2) which describe the specific orientation difference between adjacent crystals to the grain boundary and two parameters describing the spatial orientation of the grain boundary by means of the normal unit vector to the grain boundary plane $\mathbf{n}=(n_1,n_2,n_3)$ with regard to one of the adjacent grains. The other three microscopic parameters are given by the three components of the translation vector $\mathbf{t}=(t_1,t_2,t_3)$ of the displacement of one crystal with respect to the other. The intrinsic properties of the grain boundary depend on the eight parameters. In particular, the mobility and the grain boundary energy are predominantly sensitive to them.
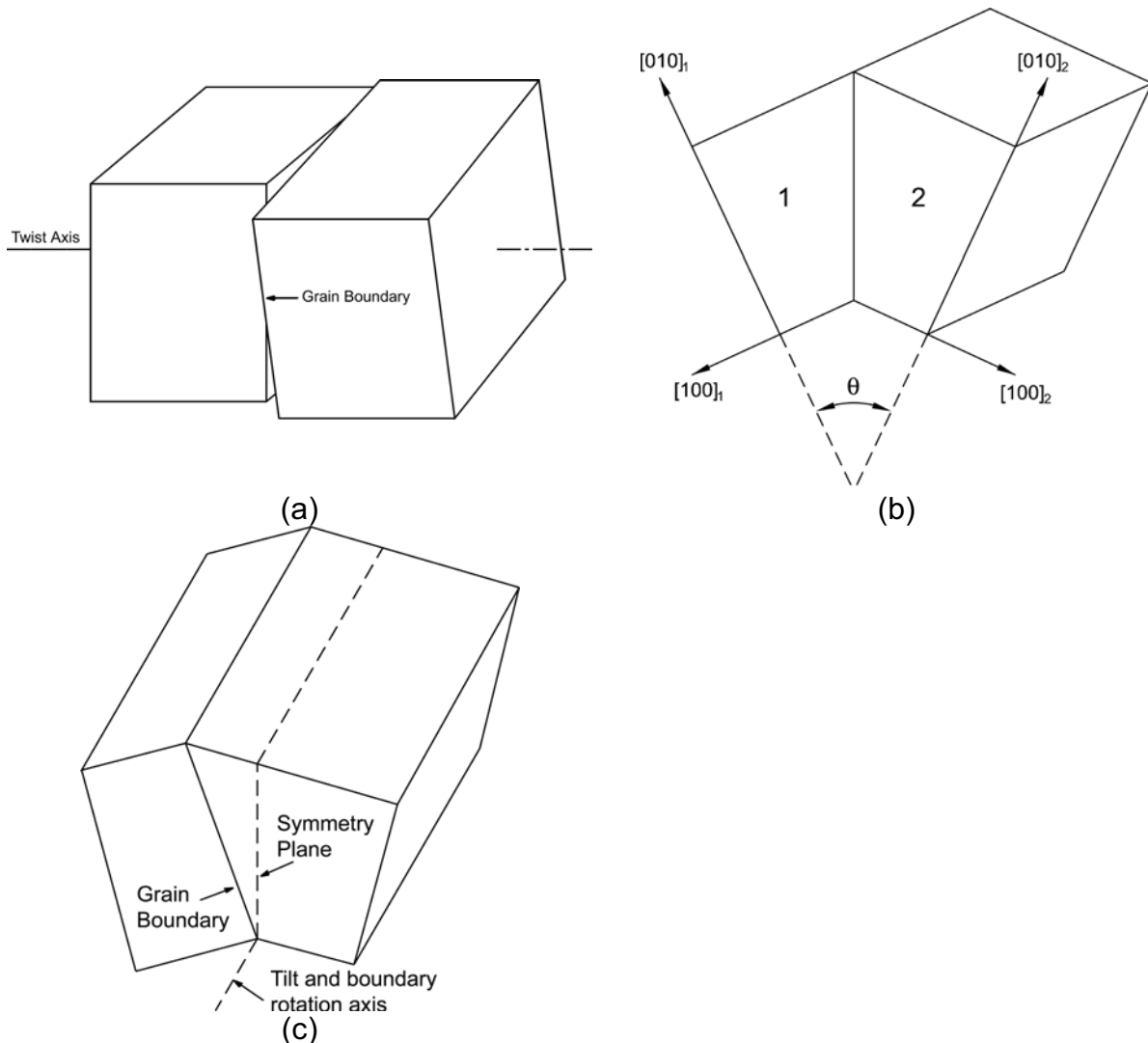
Figure 1.1. Types of grain boundaries. (a) Twist grain boundary, (b) symmetrical tilt grain boundary, (c) asymmetrical tilt grain boundary [2].

There are different kinds of grain boundaries. The easiest way to discriminate grain boundaries is to use the orientation relationship existing between neighboring crystallites. If a common origin is assumed, this relationship is reduced to a pure rotation, which can be defined in terms of a crystallographic axis *<hkl>* or a vector *[uvw]* and an angle of rotation θ. The grain boundary can now be defined using the necessary rotation to bring one of the neighboring crystallites into the orientation of the other. For example, if the grain boundary plane is perpendicular to the rotation axis, the grain boundary is referred to as a pure *twist* grain boundary (Fig. 1.1a). In contrast, if the grain boundary plane is parallel to the rotation axis, the boundary is referred to as a pure *tilt* grain boundary (Fig. 1.1b). In the case of the twist grain boundary it should be noted that the grain boundary plane is unambiguous and does not depend on the rotation angle θ, however, for the tilt grain boundaries there is not unique grain boundary plane because there is an infinite number of possible planes parallel to a given direction. The simplest type of grain boundary is the symmetrical tilt grain boundary whose boundary plane mirrors the crystallographic direction the of the adjacent crystallites. All other tilt grain boundaries are identified as *asymmetrical tilt grain boundaries* (Fig. 1.1c).

1.2.1 Low Angle Grain Boundaries

Depending on the magnitude of the rotation angle θ between adjacent crystals is also possible to distinguish two different kinds of grain boundaries: **L**ow **A**ngle **G**rain **B**oundaries (LAGB) and **H**igh **A**ngle **G**rain **B**oundaries (HAGB).
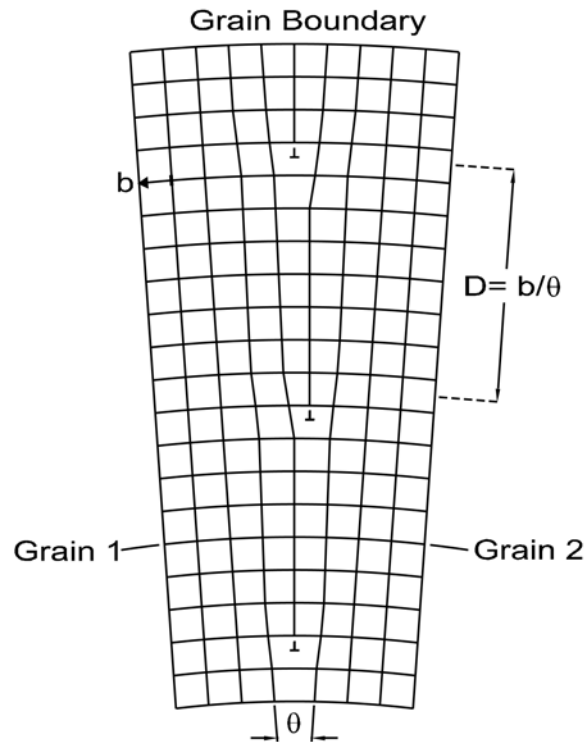

Figure 1.2. The dislocation model of a symmetrical low angle grain boundary.

A LAGB is an interface between two crystallites whose spatial orientation with respect two each other does not differ largely. This condition is reflected, precisely, in the rotation angle θ. If this angle does not exceed 15°, it is normally assumed that the grain boundary correspond to a LAGB. A LAGB is completely comprised of a periodic set of crystal dislocations. In figure 1.2, the structure of a symmetrical low angle tilt grain boundary is shown. Such grain boundary consists of one set of edge dislocations with the same Burgers vector b. The number of dislocations per unit length in the grain boundary, 1/D, increases with the misorientation angle θ

$$\frac{1}{D} = \frac{2\sin\left(\theta/2\right)}{b} \approx \frac{\theta}{b}.$$

(1.1)

In contrast, the structure of an asymmetrical grain boundary is more complex, it requires at least two sets of non-parallel edge dislocations to be constructed (Fig. 1.3). It should be noted that the grain boundary starts as a symmetrical tilt grain boundary but the increasing deviation from this configuration makes it necessary to introduce a new set of dislocations. The number of dislocations of this second set increases with increasing deviation, while the number of dislocations of the first set decreases. This situation leads to a point where the grain boundary is completely composed by dislocations of the second set. At this point the grain boundary is again

a symmetrical tilt grain boundary but perpendicular to the original grain boundary. The number of dislocations of each set can be calculated. The number of dislocations of the first set with Burgers vectors b_1 and of the second set with Burgers vector b_2 is given by

$$\frac{1}{D_1} = \frac{b_1}{\theta \cos \varphi}$$ (1.2)

and by

$$\frac{1}{D_2} = \frac{b_2}{\theta \sin \varphi}$$ (1.3)
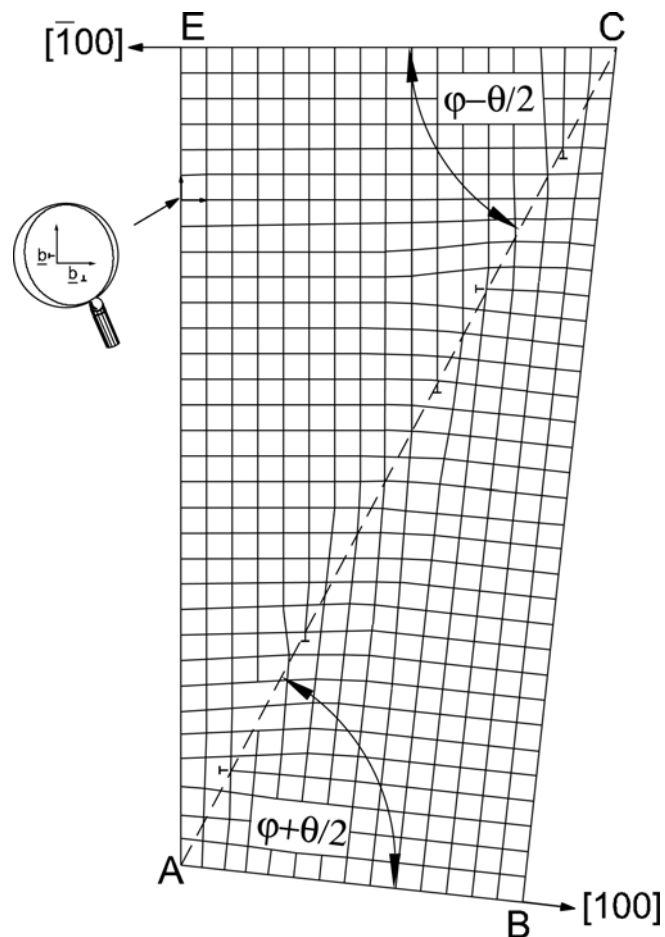
respectively.

Figure 1.3. Asymmetrical tilt low angle grain boundary [4].

The case of the low angle twist boundaries is very similar to the previous one; the only difference is that screw dislocations (Fig. 1.4) now comprise the grain boundary. These grain boundaries always require at least two sets of screw dislocations because only under this condition a rotation is generated (a single set of screw dislocation leads only to a shear deformation).
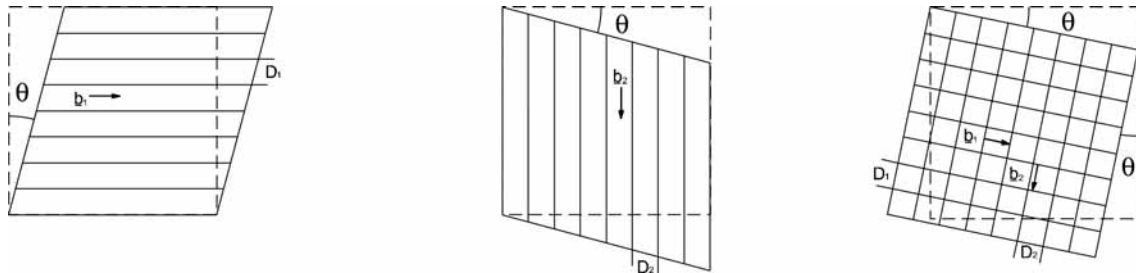
Figure 1.4. Dislocation model for a low angle twist grain boundary [2], a single set of screw dislocations lead to a shear, a second set is necessary for a rotation.

1.2.2 High Angle Grain Boundaries

For higher rotation angles ($\theta > 15°$), the dislocation model fails to describe properly the structure of the grain boundary. It can be seen from Eq. (1.1), that the number of dislocations per unit length increases with the rotation angle. However, for this equation, it is supposed that the distance between dislocations is so large that the influence of the dislocations cores can be neglected. Nevertheless, for $\theta > 15°$ the distance between dislocations reaches the range of the dislocation core radius, the dislocation cores then start to overlap and the dislocations lose their identity as individual lattice defects. Grain boundaries with rotation angles higher than 15° are called *high angle grain boundaries*. The modern understanding of the structure of these grain boundaries is still based on dislocations models of low angle grain boundaries.

The positions of the atoms of a perfect crystal are determined by the minimum of the Free Energy, the atoms will always occupy those positions that lead to this energetic state of the crystal. For the description of the structure of a high angle grain boundary, we can assume that the atoms in the grain boundary try to lie in these ideal positions (low energetic positions). If we take now two crystals with different spatial orientations and superpose them, it is possible to observe that some atoms of both crystals have the same positions; these points are referred to as coincidence sites. Due to the periodicity of the crystal lattices of both grains, the coincidence sites show also periodicity. In fact, the coincidence sites build also a lattice, which is called the **C**oincidence **S**ite **L**attice (CSL) (Fig. 1.5a). If we compare the density of a CSL with respect to the density of crystal lattice, it is possible to define the parameter Σ as follows [5]

$$\Sigma = \frac{\text{volume of elementary cell of CSL}}{\text{volume of elementary cell of crystal lattice}}. \tag{1.4}$$

This parameter defines how similar the CSL and the crystal lattice are. The larger the value of Σ is, the smaller is the number of coincidence sites in the grain boundary and vice versa. For example, a grain boundary with $\Sigma = 1$, can be found, if we consider a grain boundary which is supposedly formed between two crystals with exactly the same spatial orientation, small deviations in the orientation of one of the crystals need to be compensated by the introduction of dislocations. Even with the introduction of dislocations the grain boundary can still be considered to posses an $\Sigma = 1$ since all lattices nodes, except those of the dislocation cores, are in coincidence sites. Incidentally, this grain boundary corresponds to a LAGB.