Grain boundary in a solid crystalline material is a region separating two crystals (grains) of the same phase. These two grains differ in mutual orientations and the grain boundary thus represents a transition region, where the atoms are shifted from their regular positions as compared to the crystal interior [12, 19, 20]. Grain boundaries represent the simplest interface: If the adjoining grains differ in chemical composition and/or in parameters of the crystal lattice, the interface between them is called phase boundary (interphase boundary, heterophase boundary). The grain boundary is also called homophase boundary in this classification. In general, interfaces represent a crystallographic and/or chemical discontinuity with an average width less than two atomic diameters [21, 22] although they may be sometimes more diffuse spreading over appreciable number of interplanar spacings [12, 23]. In this context, free surface is the interface between solid and vacuum [20].

Only those aspects of grain boundaries that are necessary for further reading will be mentioned in this chapter. For more thorough information other sources are recommended to the reader, especially the comprehensive book of Sutton and Balluffi [12] and selected parts of the book edited by Wolf and Yip [24].

2.1 Crystallographic Description of Grain Boundaries

To describe grain boundary crystallographically, a number of variables must be specified. Generally, the grain boundary can fully be characterised by five independent parameters (macroscopic degrees of freedom, DOFs), which provide us with information how to prepare the bicrystal (i.e. a sample containing two grains with the required orientation of the planar separating interface) from given single crystals (e.g. [12, 22, 25–27]). Three of them specify mutual misorientation of the adjoining grains $A$ and $B$ (Fig. 2.1). This misorientation is represented by a rotation, which brings both grains in perfect matching. It is defined by the rotation axis $o$ (2 DOFs) and angle $\theta$ (1 DOF). Let us mention that there always exists at least one way how to describe such relationship in the case of non-enantiomorphic crystals. The orientation of the grain boundary between these misoriented grains is defined by the normal $n$ to the grain boundary plane (2 DOFs).
Following this characterisation, we can completely and unambiguously describe any grain boundary by the notation \( \theta^\circ[h_o k_o l_o], (h_{nA}k_{nA}l_{nA})^1 \). The grain misorientation is defined by the common axis \( o = [h_o k_o l_o] \), which is identical in both grains and expressed in a chosen co-ordinate system. The information about the grain boundary plane is related to one of these two grains only. From practical point of view, it is sometimes useful to identify the other part of the grain boundary, so that the boundary is described by \( \theta^\circ[h_o k_o l_o], (h_{nA}k_{nA}l_{nA})/(h_{nB}k_{nB}l_{nB}) \). This notation represents an over-determination, indeed, but can give an easier and quicker view on the grain boundary crystallography.

It is necessary to add that besides the above mentioned five independent macroscopic DOFs, three other microscopic parameters exist that are represented by a vector \( T \) characterising a rigid body translation of both grains relatively one to the other, parallel and perpendicular to the grain boundary plane. The latter one represents, in fact, a volume expansion [28]. These translations are independent of macroscopic DOFs but controlled by the energetic reasons and cannot be chosen arbitrarily: for each grain boundary, few mutual translations may only exist that generate equilibrium atomic structures of the grain boundary under actual external conditions such as temperature, pressure and chemical composition. Thus, they cannot be considered as independent DOFs [12, 27, 29, 30].

Five DOFs that are necessary to describe completely the crystallography of a grain boundary imply existence of a huge number of different grain boundaries. Therefore, it is sometimes reasonable to categorise the grain boundaries into groups according to the relationships among individual DOFs. For example,

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1 In case of hexagonal structures, the notation should be modified according to the corresponding description of crystal planes and directions by four Miller indices.