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On frequency of occurrence of tilt and twist grain boundaries

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Abstract

Homophase grain boundaries are frequently classified into twist–, tilt– and mixed type boundaries. With small deviations from pure twist and tilt allowed, there are finite probabilities of occurrence of these particular boundary types in a set of random boundaries. These probabilities are determined for the case of cubic crystal symmetry. If the limit on the deviations is 3 degrees, then 3.9% of random boundaries have near–twist character, and as many as 84.0% of random boundaries are near–tilt boundaries.

Keywords: Grain boundaries; Interfaces; Twin grain boundary; Coincidence site lattice (CSL)

There are a number of classifications of grain boundaries. The most basic is the distinction between low– and high angle boundaries. Then, there is a division into successive coincident lattice (CSL) boundaries and non–CSL boundaries. The third common classification is that into twist –, tilt – and mixed type boundaries [1].

One of the basic and interesting issues is to find out the frequencies of occurrence of boundaries of particular types. The frequencies for a given material can be referred to the frequencies corresponding to the random case. Hence, there is an interest in the latter numbers, i.e. in the fractions of special boundaries among random boundaries. In the cubic case, the fraction of low angle ($\Sigma 1$) boundaries defined by the $15°$ limit on the misorientation angle is 2.3%. Assuming Brandon criterion, the probabilities for the CSL misorientations of $\Sigma 3$, 5 and 7 are 1.8, 1.2 and 1.0%, respectively [2, 3]. Now, a question arises about the frequencies for the third classification: What are the probabilities for a random boundary to have twist or tilt character? To our knowledge, despite the prominence of the tilt/twist characterization, these probabilities have not been estimated before.

In contrast to CSL boundaries (including $\Sigma 1$), which are ordinarily defined based on misorientations, both misorientations and boundary plane inclinations are needed for describing twist and tilt boundaries. Until recently, the interest in examining boundary inclinations was limited because of experimental difficulties in their determination. However, this has changed with the progress in automatic serial sectioning methods and 3D characterization of materials [4, 5], and the increased activity in the areas of statistical analysis involving all five macroscopic boundary parameters (e.g., [6–8] and references therein).

Below, we calculate the frequencies of occurrence of near–twist and near–tilt boundaries among random boundaries in the case of $m3m$ (O_h) crystal point group. To introduce needed quantities, we assume that Cartesian reference systems of the same handedness are attached to crystallites. Relative orientations of the crystallites correspond to rotations relating the systems; a special orthogonal matrix, say M, can be used to represent misorientation between the first– and the second grain. To specify inclination of the boundary plane, we use a unit vector m_1 perpendicular to the plane, directed towards the second grain, with coordinates given in the coordinate system of the first crystallite. Similarly, $m_2 = -M^T m_1$, with coordinates given in the coordinate system of the second crystallite, is normal to the boundary and directed towards the first grain.

The key question is how to calculate the frequencies. One can make a rough estimation of the inequalities between fractions of special boundaries. A Σ–boundary is specified by three macroscopic parameters and two parameters are free, whereas twist boundaries are associated with three degrees of freedom and tilt boundaries are described by four continuous parameters (e.g., [1]). Hence, assuming the same limitation on deviations in all these cases, the fraction of tilt boundaries is expected to be larger than the fraction of twist boundaries, and the latter, in turn, is expected to be larger than the fractions of particular Σ–boundaries. This reasoning, however, does not indicate how big the differences can be.

To get quantitative results, a given boundary needs to be linked to its twist and tilt "components". The well known decomposition of Fortes [9] is not suitable for our purposes. We apply a method analogous to that used for estimating the frequency of occurrence of CSL boundaries [2,3]; boundaries are classified as twist or tilt boundaries if they are sufficiently close to pure twist or pure tilt boundaries. Our calculations are based on an assumed distance function in the boundary space [10][1]. The distance between the boundaries specified by (M, m_1) and (M', m'_1) equals $\sqrt{\omega^2 + (\theta_1^2 + \theta_2^2)/2}$, where ω is the angle of the rotation leading from M to M', θ_i is the angle between m_i and m'_i $(i = 1, 2)$, and $m'_2 = -M'^T m'_1$. Such a function determines a measure or model of uniformity for boundaries [10]. The fractions can be obtained by integrating this measure over regions surrounding the twist– and tilt boundaries (Fig.1). Analytical integration would be difficult due to intricacies of the boundary space and complications caused by crystal symmetry. Therefore, the problem was resolved numerically. Random boundaries were generated according to the model of uniformity following from the distance function. For each randomly generated boundary, the distances to the nearest twist and tilt boundaries were calculated via function minimization [14]. The free optimization parameters of a twist boundary were three misorientation parameters (and the boundary plane was determined by the direction of the misorientation axis). In the case of tilt boundaries, the optimization parameters were three misorientation parameters and one parameter of the boundary plane (with the second one determined by the perpendicularity of the axis and the normal to the plane). For a given boundary, all its symmetrically equivalent representations were processed, and the smallest distance was taken as the result. Finally, based on a large number of randomly generated boundaries,

Fig.1

[1]For alternative metrics, see [11,12].

the fraction of boundaries within assumed limits was counted.

It must be stressed that the symmetry is an important factor. The symmetries involved are the crystal symmetry and the interchange of the order of the crystallites [10]. This amounts to $4 \times 24^2 = 2304$ equivalent points in the product space of special orthogonal matrices representing misorientations and unit vectors representing inclinations. In a given representation, a boundary may be seen as general, but it may have an equivalent representation indicating its closeness to a special boundary[2].

As for the limitation on angular deviations, its choice might be based on arrangements of dislocation networks but expressions for such limits would be complicated. Instead, one may simply consider the limitation in relation to the accuracy of experimental measurements of boundary parameters. Since the accuracy of misorientation determination by electron backscatter diffraction (EBSD) is slightly better than one degree (e.g., [13]), and the errors for inclinations are considerably larger (e.g., [8]), we explicitly list data for tolerances of this order. Fractions for arbitrary limiting values can be read from cumulative distributions shown in respective figures.

Our results are based on 5×10^6 ($\approx 22^5$) randomly generated boundaries. The probability density function for the distances to the nearest pure twist boundary and the corresponding cumulative distribution are shown in Fig.2. The fractions of boundaries with the distance Fig.2
to a pure twist boundary not larger than 1, 2 and 3° are 0.4, 1.7 and 3.9%, respectively. The mean distance to the nearest twist boundary is 11.8°, and the median equals 11.6°. The largest registered distance to the nearest twist boundary is 28.3°.

The percentages of boundaries with the distance to the nearest pure tilt boundary not exceeding 1, 2 and 3° are 39.0, 66.3 and 84.0%, respectively (Fig.3). The mean distance to Fig.3
the nearest tilt boundary is 1.6°, and the median equals 1.4°. The largest registered distance to the nearest tilt boundary is 7.4°.

Some boundaries are concurrently close to twist– *and* to tilt boundaries [15]. The fractions of boundaries which are no further than 1, 2 and 3° from a twist– *and* a tilt boundary are 0.2, 1.3 and 3.5%, respectively.

[2]For example, the boundary on the $(1\,1\,1)$ plane with misorientation being the rotation about $[0\,1\,2]$ by 131.81° can be also expressed as the boundary with $(1\,1\,1)$ plane and tilt about $[0\,\bar{1}\,1]$ by 70.53°, or with $(1\,1\,1)$ plane and twist about $[1\,1\,1]$ by 60°.

Summarizing, the frequencies of occurrence of near–twist and near–tilt boundaries among random boundaries were determined. The work was motivated by the interest in estimating the incidence of these particular boundary types, and by the need for reference frequencies. Only the case of the $m3m$ crystal symmetry was considered (but a similar approach could be applied to other symmetries). The method was based on an assumed distance function, random generation of boundaries, and on counting boundaries within a given limit to the nearest twist– and tilt boundaries. The results confirm rough estimates of the inequalities between the frequencies of occurrence of CSL, twist and tilt boundaries. Noteworthy is the percentage of random boundaries close to pure tilt boundaries; this number turns out to be strikingly large comparing to the fractions of CSL and twist boundaries. With the current accuracy of EBSD based data, most boundaries may be interpreted as having near–tilt character.

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Captions

Fig. 1. Schematic illustration of the boundary space and the subspaces of twist– and tilt boundaries. Arrows indicate the twist– and tilt boundaries nearest to the boundary A. The boundary B is within assumed limit (marked by dashed lines) from pure twist boundaries. The fraction of twist boundaries is obtained by calculating the "volume" of the region between the dashed lines.

Fig. 2. (a) Probability density function for distances (in degrees) to the nearest twist boundary. The long tick on the abscissa marks the average distance. (b) Cumulative distribution function for the distances to the nearest twist boundary. The long tick marks the median. Disks mark the largest registered distance. The figures are drawn based on data collected in $(1/3)^{\circ}$–wide bins.

Fig. 3. Probability density function (a) and cumulative distribution (b) of the distances to the nearest tilt boundary. The graphs are based on data collected in bins of width $(1/10)^{\circ}$. Marks as in Fig.2.

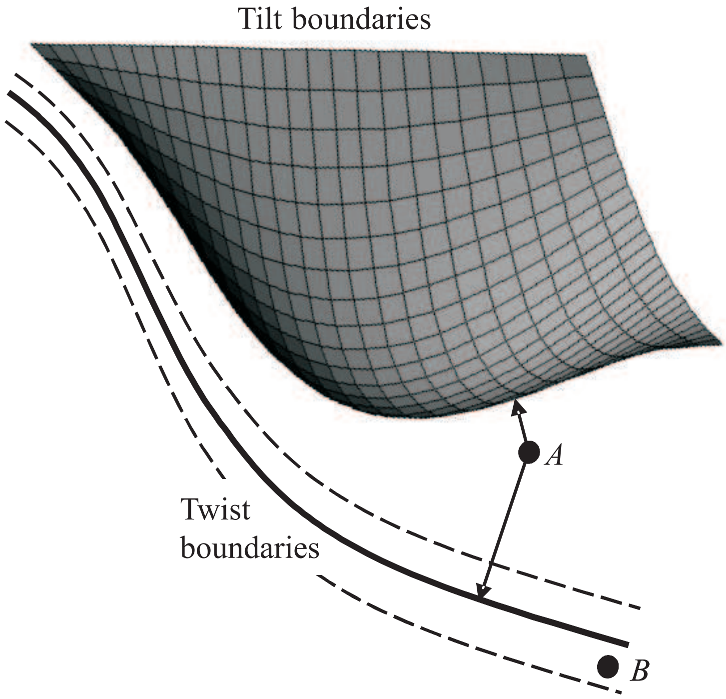

Figure 1

(Morawiec, *Frequency of occurrence of tilt and twist boundaries*)

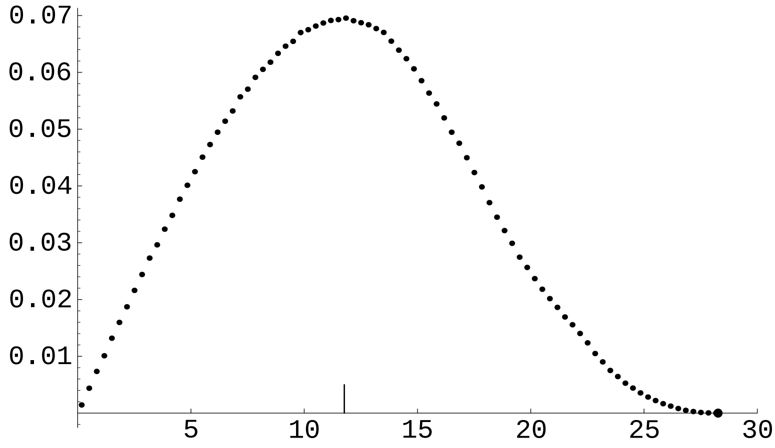

Figure 2a

(Morawiec, *Frequency of occurrence of tilt and twist boundaries*)

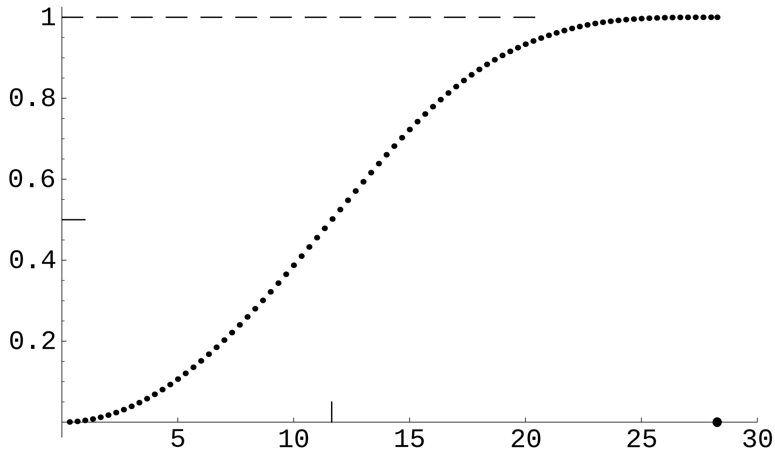

Figure 2b

(Morawiec, *Frequency of occurrence of tilt and twist boundaries*)

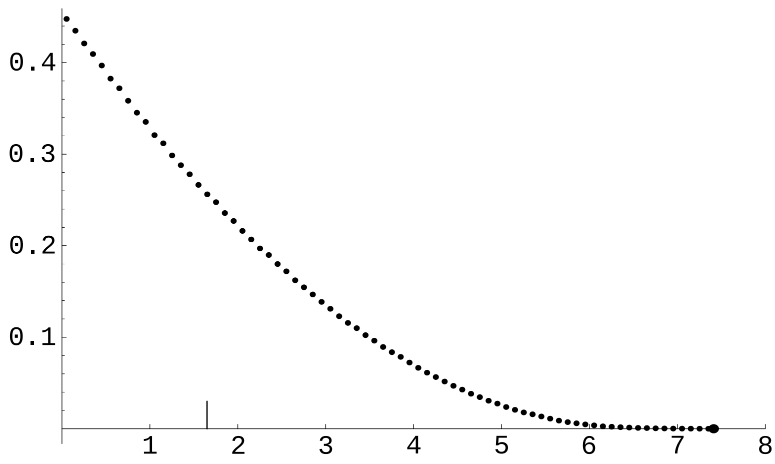

Figure 3a

(Morawiec, *Frequency of occurrence of tilt and twist boundaries*)

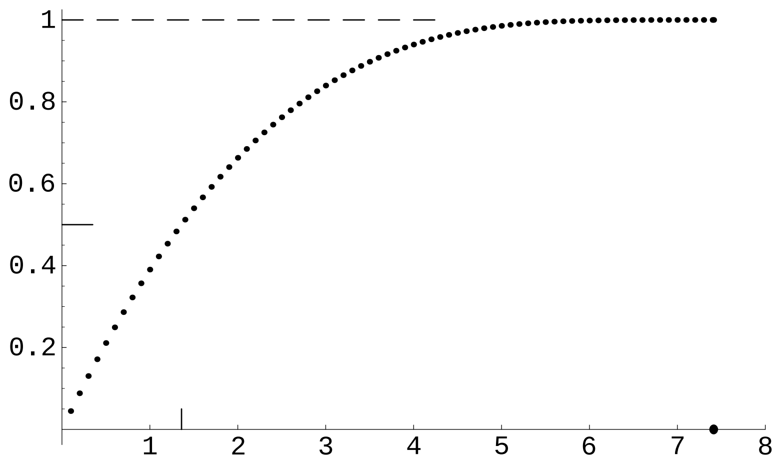

Figure 3b

(Morawiec, *Frequency of occurrence of tilt and twist boundaries*)