Comparison of experimental and predicted dislocation networks in deformation-induced dislocation boundaries aligned with slip planes in aluminium

Winther, Grethe; Huang, Xiaoxu; Hong, Chuanshi

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ABSTRACT

Deformation-induced planar dislocation boundaries aligned with slip planes in the 45° ND rotated Cube orientation in aluminium after rolling have recently been characterised in depth. In parallel the dislocation content of such boundaries has been predicted based on the Frank equation, i.e. assuming that the boundaries are low-energy-dislocation-structures (LEDS) free of long-range elastic stresses. A detailed comparison of the experimentally determined and theoretically predicted dislocation networks is presented. The comparison encompasses all the parameters in the Frank equation, i.e. the Burgers vectors, dislocation line directions, dislocation densities, misorientation and boundary plane.

1. INTRODUCTION

The deformation-induced dislocation boundaries in metals of intermediate to high stacking fault energy have been studied intensely over the past decades, partly due to their contribution to work-hardening and partly because of the scientifically intriguing process of dislocation self-assembly into a fairly regular pattern of low-angle dislocation boundaries.

The type of the dislocation structure evolving within a grain depends on the crystallographic grain orientation (Huang and Winther 2007). This grain orientation dependence has been explained by a dependence on the active slip systems (Winther and Huang 2007) leading to the expectation that the dislocations in the boundaries are those gliding on these systems. The dislocation content in a number of slip-plane-aligned boundaries in a specific grain orientation,
namely the 45° ND rotated Cube orientation, has recently been characterised (Hong, Huang and Winther 2012; Hong, Huang and Winther 2013).

According to the principle of Low Energy Dislocation Structures (LEDS), the dislocations arrange themselves in the configuration with the lowest energy that is available to them (Hansen and Kuhlmann-Wilsdorf 1986). The driving force for the assembly of dislocations in boundaries is believed to be that the dislocations screen each other’s elastic stress fields. The characteristics, i.e. Burgers vector and dislocation line, of the dislocations in a boundary free of long-range elastic stresses are related to the parameters characterising the boundary itself, i.e. the crystallographic boundary plane and the misorientation across the boundary (Frank 1950). For the 45° ND rotated Cube orientation, the dislocation networks aligned with the experimentally observed boundary plane have been derived theoretically, assuming that the dislocations move only by glide in their respective slip planes (Winther 2012). The aim of the present paper is to conduct a detailed comparison between the experimentally characterised networks and the theoretically predicted ones.

2. SLIP GEOMETRY AND BURGERS VECTOR NOTATION

For this particular grain orientation four slip systems from two slip planes are expected active but dislocations of all the six Burgers vectors of the $\frac{1}{2}<110>$ type in face-centred cubic metals were observed in the boundaries. The specific slip geometry and colour coding employed throughout the paper to designate the dislocations of the various Burgers vectors is illustrated in Fig. 1.

![Fig. 1. a) Slip system geometry in plane strain compression and b) colour coding of Burgers vectors for the 45° ND rotated Cube orientation. The two active slip planes (111) and (111̅) are coloured grey. From (C. Hong, Huang, and Winther 2013).](image)

3. EXPERIMENTAL NETWORKS

In previous papers (Hong, Huang and Winther 2012; Hong, Huang and Winther 2013) individual dislocations in a number of slip-plane-aligned GNBs in grains of the 45° ND rotated Cube orientation in 10% cold-rolled 99.996% pure aluminium were thoroughly characterised by transmission electron microscopy. The dislocations were arranged in fairly regular networks with straight dislocation lines. The Burgers vectors of all the dislocations were determined by selecting a set of diffraction conditions that made dislocations of specific Burgers vectors invisible. In addition, the line directions and densities of each type of dislocations were recorded.
The network morphologies including Burgers vectors for the five investigated GNBs aligned with the active (111) slip plane are presented in Fig. 2. While dislocations from the active slip systems with Burgers vectors $b_1$, $b_2$, $b_4$ and $b_5$ are certainly present in large densities, dislocations of the two remaining Burgers vectors are also present. In Fig. 2a dislocations of $b_3$ are found and Figs. 2b and c reveal dislocations of $b_6$. The presence of $b_3$ and $b_6$ was attributed to dislocation reactions.

![Fig. 2. Dislocation networks in the five GNBs aligned with the (111) slip plane. All scale bars represent 200 nm. Adapted from (Hong, Huang and Winther 2013).](image)

### 4. PREDICTED NETWORKS

The dislocations in a boundary that is free of long-range elastic stresses fulfill the Frank equation (Frank 1950):

$$\sum \rho_i b_i \{(n \times \xi_i) \cdot V\} = 2 \sin \frac{\theta}{2} V \times a$$  \hspace{1cm} (1)

where $b_i$ and $\xi_i$ are the Burgers vector and line direction of dislocation set i, $\rho_i$ is the planar dislocation density defined as length of dislocation line per unit area for each set. The vector $n$ is the boundary plane normal, and $V$ is any vector in the boundary plane. The symbols $a$ and $\theta$ are the crystallographic misorientation axis and angle, respectively, across the boundary.

In the previous predictions (Winther 2012) it was assumed that

- The GNB lies on the exact slip plane, i.e. $n=(111)$.
- All boundary dislocations come from one of the four slip systems expected active, i.e. only the Burgers vectors ($b_1$, $b_2$, $b_4$ and $b_5$) and slip planes ($p_x=(111)$ and $p_y=(11\bar{1})$) are considered.
- The dislocations only move by glide in their slip plane.

The main results of these predictions are summarised in the following, supplemented with new analysis results taking dislocation reactions into account.
4.1 Two sets of dislocations. With dislocations of b1 and b2 only, a twist boundary is possible, and the two sets of dislocations will react to form a regular hexagonal network of three screw dislocations, all with Burgers vectors in the boundary plane, i.e. b1, b2, and b3. This network is well-known from the literature (Hirth and Lothe 1968).

4.2 Three sets of dislocations. A network with three sets of dislocations (b1, b2 and either b4 or b5) is possible. This boundary is of mixed tilt/twist character, more specifically the misorientation axis \( \mathbf{a} \) is \([\bar{1} \ 3 \ 1]\) or \([3 \ 1 \ \bar{1}]\), depending on whether the boundary contains b4 or b5. The boundary network including b4 is illustrated in Fig. 3a, where it is seen that i) the dislocation lines of b1 and b2 are parallel, ii) b1 is a pure screw, and iii) the density of b4 is three times the density of each of b1 and b2. Dislocation reaction between b2 and b4 will produce b6 in the form of a sessile Lomer lock as illustrated in Fig. 3b. The dislocation line of the Lomer lock is given as the intersection line of the two slip planes, on which the dislocations glide, which is also the direction of the dislocation line of b4. In order to fulfil the Frank equation the dislocation line and density of b1 must also change. The network in Fig. 3b with b2 also being screws is in agreement with the equation.

4.3 Four sets of dislocations. All four sets of dislocations may also be present in the boundary, in which case it is a tilt boundary with \( \mathbf{a} = [1 \ -1 \ 0] \). All the dislocation lines are parallel to the misorientation axis, i.e. the dislocations have mixed screw/edge character. Dislocation reactions between b1 and b4 and also between b2 and b5 are possible. Both result in Lomer locks of b6 and are accompanied by changes in the dislocation lines. A network with parallel mixed dislocations of b4, b5, b6 and b1 and b2 present as screws fulfils the Frank equation.

5. COMPARISON OF EXPERIMENT AND PREDICTION

Fig. 4 is a morphological comparison of representative enlarged segments of the GNBs from Fig. 2 with the corresponding theoretical predictions. Good agreement is found in all cases:

- The morphology of the hexagonal network of GNB2 is in obvious good agreement with the theoretically predicted regular hexagonal network.
Comparison of experimental and predicted dislocation networks

- The networks from GNB7 strongly resemble the theoretical networks in Fig. 3b constructed from b1, b2 and b4 after reaction to produce b6.
- The segments from GNB3 are in corresponding good agreement with predictions with b1, b2 and b5, including dislocation reactions to produce b6.
- Fig. 4 represents two different parts of GNB4, which is not as regular as the other GNBs. In combination the two segments agree with the predicted network with all four sets of dislocations together with the Lomer locks.

In all cases the experimental dislocation line directions match the predicted ones.

![Fig. 4. Comparison of representative experimental GNB segments from Fig. 2 in circles with corresponding predicted networks in rounded boxes.](image)

The misorientation axes across the boundaries were only measured for GNB7, but for two different segments. For the remaining GNBs the misorientation axis has been calculated from the Frank equation by inserting the experimentally determined boundary plane normal, dislocation line directions and densities listed in (Hong, Huang and Winther 2013). The experimental axes agree well with the predictions as illustrated in Fig. 5. Most importantly, in each the case the experimental axis matches the axis for the corresponding predicted network in Fig. 4: GNB1 and 2 have [111] twist axes, GNB 7 and 3 have axes near [1 3 1] or [3 1 1], respectively, and finally GNB4 is close to a [1 1 0] tilt axis. The associated misorientation angles are of the order of 0.5° as also observed experimentally.

6. CONCLUDING REMARKS

The experimental and predicted networks are in good agreement, both morphologically and in terms of quantitative parameters, like misorientation, dislocation lines and densities. This proves that the GNBs are largely free of long-range elastic stresses, i.e. essentially LEDS structures. The good agreement between the calculated misorientation from the experimental dislocation densities with the predicted axes is particularly emphasised as it demonstrates that all the dislocations observed are needed, i.e. the density of redundant dislocations must be negligible.
Fig. 5. Comparison of experimentally based (red) and predicted (blue) misorientation axes. Open red circles are directly measured axes, while solid circles are calculated from the dislocation content. Two segments of GNB7 are included.

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