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COMMENTS ON THE RANGE OF APPLICABILITY OF THE GRAIN
BOUNDARY (SECONDARY) DISLOCATION MODEL TO HIGH ANGLE GRAIN
BOUNDARIES[†]

by

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COMMENTS ON THE RANGE OF APPLICABILITY OF THE
GRAIN BOUNDARY (SECONDARY) DISLOCATION MODEL TO
HIGH ANGLE GRAIN BOUNDARIES

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Introduction

In the present note we comment upon the extent to which all high angle grain boundaries can be described by the grain boundary dislocation (GBD) model which recently has been shown to apply to special boundaries having misorientations near high coincidence site density misorientations (1-3). In this model singular interfaces, which are 2-dimensionally periodic on a fine scale, and which are of relatively low energy, are formed at special high coincidence site density misorientations. Deviations from these misorientations are then compensated for by networks of discrete GBD's having Burgers vectors which are characteristic of the periodic structure of the singular interface. The structure therefore consists of a network of discrete GBD's embedded in the singular interface, with the network spacing, d , varying as

$$d \propto \frac{|\vec{b}|}{|\Delta\theta|}, \quad (1)$$

where $\vec{b}$ is the Burgers vector, and $|\Delta\theta|$ is the angular deviation from the singular misorientation. As emphasized recently (4), this model falls into the general category of a fit-misfit model with the singular interface playing the role of the region of relatively good fit and the GBD array the region of misfit.

In employing this description it is recognized of course, that all boundaries can be represented formally by arrays of dislocations (5-7). In particular, the singular interfaces for large angular misorientations can themselves be represented by uniformly and very closely spaced arrays of lattice (primary) dislocations. From this point of view the boundary consists of an array of GBD's (secondary dislocations) superimposed upon an array of closely spaced lattice dislocations (primary dislocations). However, the dislocations in the latter array are generally so closely spaced that this description has little physical significance, and it is preferable to invoke the GBD model.

The situation is rather different in the low angle regime, since here the

primary dislocations making up the singular interfaces are well separated and physically distinguishable. In addition, it is readily shown that the (secondary) GBD's actually represent periodic disturbances in the otherwise uniform spacing of the primary dislocations (5,8). Since the primary dislocations are distinguishable, it seems most reasonable to regard such boundaries as composed of arrays of discrete lattice dislocations which possess small errors in periodicity when the misorientation differs from a singular misorientation.

In the present note we are concerned with the fraction of all high angle boundaries which can be "well represented" by an array of discrete GBD's embedded in a singular interface which is periodic on a fine scale, i.e., of the order of a few atomic distances or so. We shall regard a boundary as "well represented" whenever the GBD spacing is at least twice the wavelength of the singular interface. This somewhat arbitrary criterion insures the periodicity of the interface which is presumably the cause of its relatively low energy. We are interested in short wavelength interfaces, since we intuitively expect the energy to increase with wavelength, and alternative structures may become more stable when the wavelength becomes too large. In addition, the magnitude of the GBD Burgers vectors decreases with increasing wavelength (see below), and the GBD description is therefore of relatively little physical interest when the wavelength becomes overly large, and the Burgers vector becomes exceedingly small.

As seen from equation (1), when the deviation $|\Delta\theta|$ becomes sufficiently large, the GBD's tend to overlap, and the model tends to break down. However, there are many singular misorientations distributed throughout 3-dimensional "misorientation space", and at this juncture another singular misorientation may be present nearby which will allow the structure to adopt a new and suitable GBD configuration. There is a question at present about whether enough singular misorientations of sufficiently short wavelength are available, and whether the regions of deviation centered around these singular misorientations are sufficiently extensive, to allow boundaries of all misorientations to adopt suitable GBD configurations. This question is difficult to answer either experimentally or theoretically. The predicted Burgers vectors of many of the GBD's are relatively small, and the GBD spacings should often be exceedingly fine. Consequently, the GBD's will usually not be detectable by standard transmission electron microscopy (3,9,10). Theoretically, it is difficult to estimate which of the large number of conceivable GBD type interfaces will be stable.

Brandon (1) and Fletcher (11) have estimated that ~40% of all crystal orientations could be connected by GBD type boundaries in cubic crystals by making the somewhat arbitrary assumption that Σ , the reciprocal coincidence density, cannot exceed 20. As shown below, the wavelength of the singular interface tends to increase with increasing Σ . However, additional assumptions have been made in this estimate, and the result is therefore highly questionable. More recently Warrington (2) has carried out a more refined calculation based on $\Sigma \leq 25$ and estimates

that only ~18% of all boundaries would be of the GBD type.

In the present note we wish to focus attention on the following two factors, both of which tend to increase the range of applicability of the GBD model, and both of which have been ignored previously in the published literature:

(1) For each singular interface there is a hierarchy of GBD Burgers vectors of continuously increasing magnitude which possibly may be pressed into service in order to stabilize GBD type boundary structures.

(2) There are considerable numbers of misorientations which give rise to near-coincidence situations in the boundary plane. A high coincidence site density situation can then be achieved over large patches of the boundary by introducing a suitable network of misfit GBD's. The result is a GBD type boundary which is quite similar to that which is achieved when the misorientation is close to an exact coincidence misorientation. This result has been first pointed out explicitly by Bishop et al. (13) in as yet unpublished work.

On the Hierarchy of GBD Burgers Vectors

In order to be specific, consider the series of pure high angle twist boundaries in the fcc system which is produced by rotation around [001]. High coincidence conditions are obtained at a number of singular rotations, θ_s , and networks of orthogonal screw GBD's have been observed in gold (3,9) in the vicinities of $\theta_s = 22.6, 28.1$ and 36.9° corresponding to $\Sigma = 13, 17$ and 5 as indicated in Fig. 1 (see caption) and the Table. It seems highly likely that observational difficulties limited the angular range over which networks of discrete GBD's

FIG. 1

Observed GBD spacing, d , versus twist angle, θ , for high angle [001] twist boundaries in gold. Circles represent spacings measured by electron microscopy (9). Triangles represent cases where GBD's not detected. Dashed hyperbolas calculated from equation (1).

were detected (3,9,10), and in the following we suggest that they may actually

TABLE

Data for the Screw GBD Networks Which Possess the Three Sets of
Smallest Possible Burgers Vectors in $\Sigma = 5, 13$ and 17 Type
Pure [001] Twist Boundaries

θ_s (deg)	Σ	$b_1(\text{\AA})$	$ \Delta\theta_1 $ (deg)	$d_1(\text{\AA})$	$b_2(\text{\AA})$	$ \Delta\theta_2 $ (deg)	$d_2(\text{\AA})$	$b_3(\text{\AA})$	$ \Delta\theta_3 $ (deg)	$d_3(\text{\AA})$
22.6	13	0.80	0→2.2	∞→20.8	1.13	2.2→3.1	29.4→20.8	1.60	3.1→4.4	29.4→20.8
28.1	17	0.70	0→1.7	∞→23.8	0.99	1.7→2.4	33.6→23.8	1.40	2.4→3.4	33.6→23.8
36.9	5	1.29	0→5.7	∞→12.9	1.82	5.7→8.1	18.2→12.9	2.58	8.1→11.4	18.2→12.9

exist over the entire twist misorientation range.

Consider first the $\Sigma=5$ boundaries in the vicinity of $\theta_s = 36.9^\circ$. The three smallest sets of possible Burgers vectors for these boundaries, $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$, are indicated in Fig. 2a where the section of the DSC-lattice* parallel to the

FIG. 2

Unrelaxed misfit across $\Sigma=5$ (a) and $\Sigma=13$ (b) [001] singular twist boundaries. One cell of coincidence lattice shown in each case. DSC-lattices also shown.

plane of the boundary is shown. Experimentally it has been shown (9) that networks possessing the Burgers vector $\vec{b}_1$ are present in the angular range $0^\circ < |\Delta\theta_1| \leq 1.65$ in agreement with our expectation that the array with the smallest possible Burgers vector should be present. This expectation is based on the result that the boundary energy may be written as

$$E = E_s + E_{sd} + b[A|\Delta\theta| + B|\Delta\theta|\ln(1/|\Delta\theta|)], \quad (2)$$

where E_s is the energy of the singular interface, E_{sd} is the interaction energy between the GBD network and the singular interface, and the third term is the energy of the screw GBD network where A and B are independent of $|\Delta\theta|$ (3,5). According to equation (2), the energy is generally minimized by choosing the GBD network with the smallest possible Burgers vector. Beyond $|\Delta\theta_1| = 1.65^\circ$ no net-

* The DSC-lattice, which is described in detail by Bollmann (2), gives all possible Burgers vectors for a given singular boundary.

works have been detected presumably because of experimental difficulties, and it is interesting to speculate upon possible GBD structures in this range. As $|\Delta\theta_1|$ increases beyond 1.65° the GBD spacing should decrease until it becomes equal to about twice the wavelength, λ , of the singular interface causing breakdown of the model as discussed previously. This would occur at a spacing of

$$d \approx 2\lambda = 2\sqrt{\Sigma}b_0, \quad (3)$$

since $\lambda = \sqrt{\Sigma}b_0$, where $b_0 = |a/2\langle 110 \rangle| = 2.89\text{\AA}$ (see Fig. 2). Since $\vec{b}_1 = b_0/\sqrt{\Sigma}$, this point is reached at the deviation

$$|\Delta\theta_1| = \frac{1}{2\Sigma}, \quad (4)$$

which in this case is 5.7° (see Table) and which is considerably larger than the limit of observation of 1.65° . At this juncture it seems conceivable that the boundary might re-establish a new GBD network using the next largest possible Burgers vector (i.e., $\vec{b}_2$) in order to produce a new and stable boundary structure possessing a larger GBD spacing. According to this suggestion the relatively low energy singular interface would act to stabilize the new GBD array with the increased Burgers vector. As seen in the Table, this structure might then be stable over the angular deviation range $5.7^\circ \leq |\Delta\theta_2| \leq 8.1^\circ$ until it would be supplanted by another network possessing the larger Burgers vector $\vec{b}_3$ which would be stable over the range $8.1^\circ \leq |\Delta\theta_3| \leq 11.4^\circ$. We note, of course, that these structures would only be stable if they possessed lower energies than other conceivable alternative boundary structures. We estimate that none of the GBD networks in these proposed boundaries would be readily visible by standard transmission electron microscopy primarily because of their small spacings (see Table). The existence of these suggested boundaries is therefore not inconsistent with any available experiments.

Similar considerations hold for the other boundaries based on the $\Sigma=13$ and 17 interfaces. The hierarchy of possible sets of Burgers vectors for the $\Sigma=13$ interface is shown in Fig. 2b. A summary of GBD data for the three smallest sets of Burgers vectors for each boundary is given in the Table. It is noted that GBD boundaries of the type listed in the Table provide complete coverage of the angular range in the high angle regime (Fig. 1). It should also be mentioned that even larger Burgers vectors (including lattice vectors) could be invoked in certain cases.

Near-Coincidence Type GBD Boundaries

Several near-coincidence misorientations occur in the range of twist angles considered in the previous section. An example is given in Fig. 3 where the rotation is 31.0° around $[001]$. The square cells in the (001) planes of the two crystals which almost match at this misorientation are shown in Figs. 3a,b. The mismatch corresponds to a uniform dilatational strain (without rotation) of $\epsilon = 0.028$ in the (001) plane. The matched planes after dilatation and superposition

FIG. 3

Misfit across $\Sigma=17$ near-coincidence [001] twist boundary at $\theta=31.0^\circ$. (a) and (b) show almost matching planes before joining. (c) shows unrelaxed misfit after joining. Two-dimensional DSC-lattice is indicated.

are shown in Fig. 3c and are seen to form a 2-dimensional coincidence lattice in the plane of the boundary of wavelength $\lambda \approx \sqrt{17} b_0 \approx 12\text{\AA}$. The 2-dimensional DSC lattice which is produced is also shown along with possible sets of Burgers vectors. In this case the long range dilatational strain can be cancelled by introducing an array of orthogonal edge GBD's having Burgers vectors of the type $\vec{b}_1$ ($b_1 = 0.68\text{\AA}$) and a spacing $d = b_1/\epsilon \approx 24\text{\AA}$. The result is a GBD type boundary which consists of an orthogonal array of edge GBD's embedded in the relatively short wavelength periodic interface shown in Fig. 3c. (We note that we have barely satisfied our criterion that $d \approx 2\lambda$ in this example. This situation could be alleviated by choosing edge GBD's with larger Burgers vectors of the type $\vec{b}_2$ (Fig. 3c) as suggested in the previous section).

No experimental evidence for the existence of this type of boundary, whose orientation falls in between those of the $\Sigma=17$ and $\Sigma=5$ boundaries, has been found as seen in Fig. 1. One explanation for this result is that an alternative boundary structure has lower energy as discussed previously. Another explanation is that boundaries of this type actually exist near $\theta=31^\circ$ but that the GBD struc-

ture has not been detected. The edge GBD array present at $\theta_s = 31.0^\circ$ is finely spaced ($24\text{\AA}$) and possesses a small Burgers vector ($b_1 = 0.68\text{\AA}$). Small deviations from θ_s would presumably be accommodated by GBD's with Burgers vector $\vec{b}_1$, and again it is quite possible that they would have escaped detection.

We are currently identifying additional near-coincidence misorientations and are carrying out a further investigation of the geometry of near-coincidence type boundaries in the fcc structure.

Concluding Remarks

We have suggested that GBD networks possessing the hierarchies of Burgers vectors which are possible in singular interfaces may lead to stable GBD type high angle grain boundaries and hence be responsible for extending the range over which such boundaries exist. In addition, near-coincidence situations exist which may also give rise to stable GBD type boundaries and further extend the range of boundaries of this type. We therefore conclude that the range of applicability of the GBD model may be wider than previously supposed (1,11,12). It appears that a lack of experimental resolution has restricted the observation of many GBD type boundaries. There is current need for high resolution experimental work and also theoretical calculations to investigate the range of existence of such boundaries further.

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