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Continuous Distribution of Dislocations in Intercrystalline Boundaries

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The structure of a dislocation network in a crystal boundary depends, among other parameters, on the two crystal structures and their relation, *i.e.* the linear transformation leading from one crystal lattice to the other. For the same transformation, the structure of the network is related to the crystal structure. The link between the transformation and the many possible dislocation networks is described by a theorem which states that the displacement field of the linear transformation in the boundary can be described in an infinite number of ways by continuous dislocation distributions. The discrete dislocations are then obtained by grouping the continuous dislocations. The *O*-lattice theory is discussed in relation to these new aspects, particularly with respect to the features which tend to be conserved in the boundary. A special discussion is given of the case where a common crystallographic axis, without the relaxation pattern being periodic, represents the preferred state.

1. Introduction

Two crystals joined at a boundary can be considered as being geometrically related by a linear transformation, which, in the general case, consists of a translation part plus a homogeneous transformation, such as for example a rotation, shear, expansion *etc.* We discuss for the moment the homogeneous part and investigate transformations which conserve the number of dimensions, *i.e.* those which image a three-dimensional space (crystal) again in three dimensional space. Hence, projections are excluded.

A homogeneous transformation leaves the origin unchanged. Outside the origin it produces a 'displacement field'. Any point, situated where it was before the transformation had acted (starting point), is related to a point after that action (end point). The field of all the vectors from the starting point to the end is the 'displacement field'.

By means of the *O*-lattice method [(Bollmann, 1970, further referred to as (I)] a boundary between two crystals can be represented by a dislocation network. The problem of the present paper is to find the link between the continuous displacement field and the discrete dislocation network in the boundary. Take the case of the displacement field of a small rotation (twist boundary); this displacement field is unique and well defined. However, depending on the crystal structure, the dislocation network can be square, hexagonal, rectangular, *etc.* We shall show that the link between the displacement field and the dislocation network is given by the possibility of representing the displacement field as combinations of continuous dislocation distributions. The discrete dislocation network is then achieved by grouping the continuously distributed dislocations.

Once this relation between displacement field and dislocation network is established, the *O*-lattice method will be discussed from this new point of view.

A theory of continuous dislocation distributions has been developed among others by Bilby, Bullough & Smith (1955), and by Kröner (1958). The present approach has been developed independently of that work.

2. Theorem of continuous dislocation distributions

2.1. *The displacement field*

The displacement field (**T**) of a homogeneous linear transformation **A** [rank (**A**) = 3] can be represented either with respect to the starting point (*s*) [(*f*) = final point)]:

$$\mathbf{x}^{(f)} = \mathbf{A}\mathbf{x}^{(s)} \tag{2.1}$$

$$\mathbf{T}^{(s)} = (\mathbf{A} - \mathbf{I}) \tag{2.2}$$

$$\mathbf{x}^{(s)} + (\mathbf{A} - \mathbf{I})\mathbf{x}^{(s)} = \mathbf{x}^{(f)}, \tag{2.3}$$

or with respect to the final point (*f*):

$$\mathbf{T}^{(f)} = (\mathbf{I} - \mathbf{A}^{-1}) \tag{2.4}$$

$$\mathbf{x}^{(f)} - (\mathbf{I} - \mathbf{A}^{-1})\mathbf{x}^{(f)} = \mathbf{x}^{(s)}. \tag{2.5}$$

This second representation is needed in the *O*-lattice theory and will be used throughout this paper.

2.2. *The meaning of a continuous dislocation distribution*

As is well known, a moving dislocation line acts as a translation operator. The Burgers vector, the sign of which is related to the line sense, can be represented as:

$$\mathbf{t}^{(i)} = \mathbf{u}_k^{(i)} b^k \quad (i = 1,2;\ k = 1.2.3) \tag{2.6}$$

where $\mathbf{t}^{(i)}$ is a translation vector either in crystal 1, ($i = 1$) or in crystal 2 ($i = 2$). The $\mathbf{u}_k^{(i)}$ are the three unit vectors of the respective crystal unit cell, and b^k are the dimensionless coordinates of the translation vector. These coordinates are those which are conserved in dislocation reactions and hence form 'the Burgers vector', while the vectors $\mathbf{t}^{(i)}$ are the 'local representa-

tions of the Burgers vector' in either crystal (Bollmann, 1974). The movement rule [(I), p. 48] can be formulated for a dislocation moving in a grain boundary, in the following way.

A moving dislocation separates the space virtually into two parts and translates one part with respect to the other. If **l** is the line sense and **v** is a vector pointing in the direction of the dislocation movement, the vector **m**:

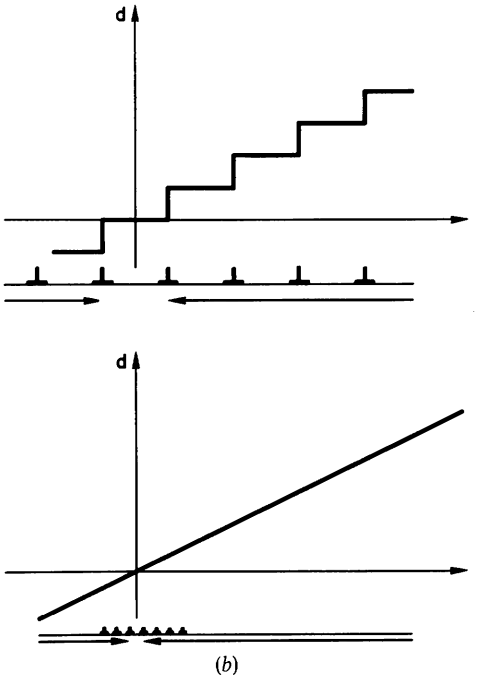
$$\mathbf{m}=\mathbf{l}\times\mathbf{v} \tag{2.7}$$

marks that part which is translated by its local representation of the Burgers vector, while the other part is kept fixed.

Hence, a moving dislocation produces a relative shift in its wake, up to the location where it stops. A further dislocation produces an additional displacement up to its end position, *etc.* Hence, a series of dislocations produces a stepwise displacement, Fig. 1(*a*).

A continuous displacement can be considered as a limiting case of the discrete sequence of dislocations, where the dislocation spacing as well as the Burgers vectors become infinitesimal. Here, the Burgers vector has to be defined as displacement per unit band width of dislocations, Fig. 1(*b*). The proposed theorem is now the following.

Theorem. The displacement field in an interface between two bodies, the orientation and structure of which are related by a homogeneous linear transformation, can be represented in an infinite number of ways by the action of different continuous distributions of infinitesimal dislocations.



(*b*)

Fig. 1. (*a*) Displacement, *d*, as introduced by incoming dislocations. (*b*) Displacement produced by a continuous set of dislocations.

The displacement field produced by one continuous distribution of straight, 'equally spaced' dislocations between the state before the dislocations have been present and that after the dislocations have run-in from both sides up to the origin is actually the displacement field of a general shear transformation. This shear transformation leaves an undisplaced line (plane) through the origin and produces a displacement proportional to the distance from that line (plane). Hence, the proof of the theorem is to show that the displacement field of any dimension-conserving homogeneous linear transformation can be represented in an infinite number of ways as different sums of displacement fields of shear transformations.

The general form of a shear transformation is

$$h_k^i=\delta_k^i+v^i n_k \tag{2.8}$$

with δ_k^i = unit matrix, v^i = shear vector, n_i = shear plane normal (unit vector).

The inverse shear transformation is a shear too, with the same shear plane and the shear vector w^i:

$$w^i=\frac{-v^i}{(1+v^k n_k)}. \tag{2.9}$$

The Einstein convention is applied here which states that, if in a product the same index (k) appears in the upper and the lower position, the product is to be summed over that index

$$v^k n_k \equiv \sum_{k=1}^{3} v^k n_k = v^1 n_1 + v^2 n_2 + v^3 n_3 . \tag{2.10}$$

The displacement field of a shear transformation (which we abbreviate to the term 'shear field'), given by $(\mathbf{I}-\mathbf{H}^{-1})$ (referred to the end point of the displacement vector) has the form:

$$d_k^i = w^i n_k . \tag{2.11}$$

Hence, in a two-dimensional case, in matrix form the decomposition of the displacement field of the given linear transformation **A**, *i.e.* of $\mathrm{T}=(\mathbf{I}-\mathbf{A}^{-1})$ into two shear fields is given by:

$$\begin{pmatrix} w_1^1 n_1^1 & w_1^1 n_2^1 \\ w_1^2 n_1^1 & w_1^2 n_2^1 \end{pmatrix} + \begin{pmatrix} w_2^1 n_1^2 & w_2^1 n_2^2 \\ w_2^2 n_1^2 & w_2^2 n_2^2 \end{pmatrix} = \begin{pmatrix} t_1^1 & t_2^1 \\ t_1^2 & t_2^2 \end{pmatrix} \tag{2.12}$$

with w_m^i the ith component of the mth shear vector and n_k^m the kth component of the mth shear-plane normal.

In the general index notation the decomposition becomes:

$$w_m^i n_k^m = t_k^i . \tag{2.13}$$

This expression, however, can also be interpreted as the following matrix product:

$$\left(\begin{array}{c|c} w_1^1 & w_2^1 \\ w_1^2 & w_2^2 \end{array}\right) \left(\begin{array}{cc} n_1^1 & n_2^1 \\ \hline n_1^2 & n_2^2 \end{array}\right) = \begin{pmatrix} t_1^1 & t_2^1 \\ t_1^2 & t_2^2 \end{pmatrix} \tag{2.14}$$

where the column vectors of the first matrix are the shear vectors $\mathbf{w}_m$ and the row vectors of the second matrix the shear-plane normals, $\mathbf{n}^m$, which shows that

the shear vectors and the shear-plane normal can be collected in different matrices.

In the general three-dimensional form the indices i and k can acquire the values $i=1,2,3$ and $k=1,2,3$ and the index m can be an arbitrary number. Then the matrix **W** with m columns and three rows is multiplied by the matrix **N** with three columns and m rows. If the shear planes (vectors **n**) are given, and hence the matrix **N**, (2.14) furnishes nine equations for the $3m$ unknown components of the shear vectors.

The compatibility of the equations has to be studied for each case. For example, if a rotation field is represented by two shear fields the shear planes have to pass through the rotation axis. If, however, it is represented by three shear fields with non-coplanar normal vectors, the shear vectors $\mathbf{w}_m$ prove to be coplanar on the plane perpendicular to the axis of rotation. They are uniquely determined. Further, a decomposition of a rotation field into three shear fields with the shear planes passing through the rotation axis leaves the freedom of choice of one of the shear vectors, where the shear vectors do not have to be coplanar.

The minimum number of shear fields needed to compose the displacement field of a linear transformation **A** is the rank of **T**, *i.e.* for example, if **A** is a three-dimensional expansion, then at least three shear fields are needed. For a rotation two of them are sufficient and the case of **A** being a shear transformation is trivial. However, even a shear field can be composed of several other shear fields. An example of the decomposition of a rotation field into two shear fields and hence into two continuous dislocation sets is given in Appendix *A* and Fig. 2.

We do not explore the problem mathematically to its limits. The statement of the theorem is proved by showing that there exists actually an infinite multitude of decompositions of a field of a linear transformation into shear fields because of the freedom of choice of the shear planes and eventually also shear vectors.

The displacement field of a transformation **A** is three-dimensional and so are the shear fields. The continuous dislocation distribution, however, comes into being the moment an interface is chosen, where one side of the interface is in the starting position and the other side in the final position of **A**. The sign of the dislocations, *i.e.* the coupling between the line sense and the orientation of the Burgers vector is determined by which side of the interface is chosen for crystal 1 (and for crystal 2, respectively).

In the case of a non-homogenous transformation, the translation part is represented by a dislocation which has swept the whole area of the interface and hence has translated one crystal with respect to the other in addition to the remaining continuous dislocation distribution which represents the homogeneous part of the transformation. It is to be expected that the theorem will also hold for 'locally linear' distorted transformations. Here, however, the 'continuous' dislocation sets will not be straight and will no longer be of constant density.

We shall now discuss the *O*-lattice theory in the light of our theorem.

3. Discussion of the *O*-lattice theory with respect to the continuous dislocation distributions

It is to be pointed out at the beginning that the mathematical machinery of the *O*-lattice theory [as given in (I)] stays unchanged by these new aspects. However, the whole context becomes wider and more transparent.

The *O*-lattice theory, which is a geometrical theory

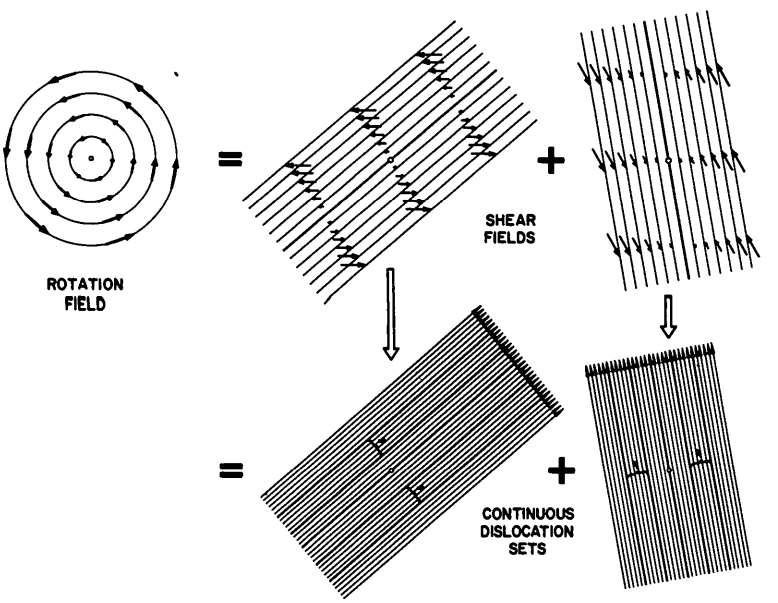


Fig. 2. Decomposition of a rotation field into two shear fields and correspondingly into two continuous sets of dislocations.

of the structure of intercrystalline boundaries, is applied on two levels, which are distinguished by the local conservation of certain structural features. On the primary level it is the crystal structure itself which is locally conserved and on the secondary level it is a whole relaxation pattern.

3.1. *The primary level*

In order to make our ideas more concrete we discuss the problems with examples.

As a first example, we imagine the case of a twist boundary, ($\theta = 10°$, [001]), in the hexagonal structure with lattice constant a. The standard O-lattice procedure is to start with the perfect crystal, formulate the transformation **A** (the 10° rotation), then solve the O-lattice equation

$$(\mathbf{I} - \mathbf{A}^{-1})\mathbf{x}^{(0)} = \mathbf{b}^{(L)} \tag{3.1}$$

[$\mathbf{b}^{(L)}$ means lattice vectors of the b lattice] where in our case $\mathbf{b}^{(L)}$ are the unit vectors of the hexagonal structure $\{a(100)$ and $a(-\frac{1}{2}, \sqrt{3}/2, 0)$ in b subspace [(001) plane]$\}$.

The solutions are O lines in the **z** direction with the xy positions (column vectors):

$$\mathbf{X}^{(0)} = \left(\begin{array}{c|c} (a/2) & (3a/4)\cot(\theta/2) - (a/4) \\ -(a/2)\cot(\theta/2) & (a/4)\cot(\theta/2) - (3a/4) \end{array}\right)$$

and all their linear combinations. (For the positions of the O lines see Fig. 3.) These O lines are separated by bisecting cell walls. The cut of the boundary with the cell walls represents the dislocation network, the Burgers vectors of which are attributed from the b net by means of the duality relations [(I), §9.1].

From the new point of view we imagine the situation in the following way: we assume the bicrystal to be in the actual state, the 10° twist, the type of boundary not yet being decided. The crystal now 'feels around' for some energetically preferred state and finds it to be the state of the perfect crystal, which would be attained by a $-10°$ rotation (of crystal 2). However, the crystal cannot twist, so it changes the twist from the preferred state to the actual state into a continuous dislocation distribution, such that the neutral lines come to lie parallel to the O-lattice unit vectors. The preferred state, the state of the perfect crystal, is optimally realized at the O elements (coincidence of equivalent positions). Then, the continuous dislocations become grouped into discrete dislocations between the rows of O points. It is like curtains being drawn apart and packed between the rows of O points, these packed curtains being the discrete dislocations. The uncovered 'windows' around the O points up to the dislocations show now the energetically preferred state, *i.e.* the state of the perfect, albeit somewhat elastically distorted, crystal (Fig. 3). The O-lattice procedure guarantees that the Burgers vectors of the now discrete dislocations are translations which conserve the state of the perfect crystal, *i.e.* they are translation vectors of the perfect crystal. The O-lattice equation (3.1) shows that the O element is located at the tip of a vector of the displacement field of **A**, which is a translation vector conserving the state of the perfect crystal (crystal 1).

The dislocation network which is needed for the local conservation of the structure of the perfect crystal is the 'primary' dislocation network. The parts

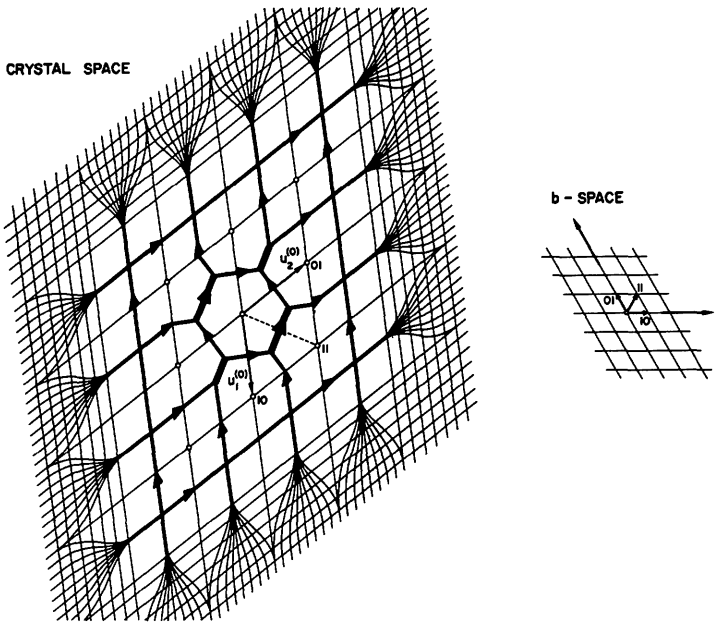


Fig. 3. Grouping of continuous dislocations to form discrete ones and forming dislocation reactions. The picture is an illustration of the idea rather than a description of the actual process, while the latter is considered to be instantaneous.

of the O elements (O points, O lines, O planes) in the boundary are the locations where this structure is optimally conserved. The primary dislocation network, as closely spaced as it may be, is essentially always present. It dominates the relaxation in the boundary. For a discussion on relaxation see Appendix *B*.) It may happen that for large deviations in the relative orientation, different unit cells in the two crystals have to be chosen so that the transformation **A** becomes a combination of a unimodular transformation with a rotation, or in phase boundaries the relation may be different again, but all these transformations can be represented in an infinite number of ways by continuous dislocation distributions where the conserved (preferred) structure picks out the appropriate distribution and groups the continuously distributed dislocations into discrete dislocations.

To summarize: instead of starting with the perfect crystal and forming the actual state of the bicrystal, we conceptually start with the actual bicrystal and 'locate' the state of the perfect crystal. The displacement field of the transformation (**A**) which is needed to attain the actual state, starting from the preferred state, represents an infinite number of virtual continuous dislocation distributions. The locations where the perfect crystal is best realized in the boundary (O elements) and the translations which reproduce the structure of the perfect crystal (b lattice) determine the choice of the appropriate continuous dislocation distribution. The discrete dislocation network is then obtained by grouping the continuously distributed dislocations between the O elements.

Hence, the dislocation network is an intermediate state between: (*a*) the state of two crystals put together without any atomic forces acting (continuous displacement field) and (*b*) the state of the perfect crystal, which would be fully attained if all the dislocations had run out of the boundary.

3.2. *The secondary level*

3.2.1. *The conservation of a coincidence pattern*

While on the primary level the crystal structure itself is locally conserved, the secondary level is determined by the local conservation of a whole relaxation pattern, *e.g.* a coincidence pattern. [For recent experimental evidence of the existence of coincidence patterns see Herrmann, Gleiter & Bäro (1976).] The O-lattice procedure is exactly the same as on the primary level, only the crystal lattices are replaced by DSC lattices (see below), and the relative orientation of the crystals is replaced by the deviation from the coincidence orientation [Warrington & Bollmann (1972)].

When two crystals are in a coincidence relation, the pattern formed by the lattice points is periodic with the period determined by the coincidence sites ($\Sigma=13$ means that the period contains 13 crystal units). If crystal lattice 2 is translated with respect to crystal lattice 1, the size of the period will remain the same, but the motif of the pattern will change. Certain specific translations, however, will reproduce the motif of the departure. The DSC lattice is formed by all those translations which reproduce the configuration of the starting motif. The DSC lattice is also called the 'complete pattern shift lattice', where D stands for displacement of crystal lattice 2 with respect to crystal lattice 1, S for shift of the pattern and C for complete. While the points of the coincidence site lattice are contained in both crystal lattices, the DSC lattice is a lattice which contains both crystal lattices (Fig. 4). The translation vectors of the DSC lattice are possible Burgers vectors of secondary dislocations. The DSC lattice is closely related to the reciprocal coincidence site lattice (Grimmer, Bollmann & Warrington, 1974; Grimmer, 1974).

The procedure for determining the secondary dislocation network starts with the DSC lattice 1, into which crystal lattice 1 is embedded, and the DSC lattice 2 which contains crystal lattice 2. In the coincidence orientation the two DSC lattices coincide. The situation is fully analogous to that of the perfect crystal. On deviation from coincidence orientation, the DSC lattice 2 deviates in orientation from DSC lattice 1. Here again the displacement field of that deviation can be decomposed into the appropriate sets of continuous dislocations and located and bundled according to the O-lattice procedure. The Burgers vectors are in this case vectors of the DSC lattice.

Since the translation vectors of both crystals are always contained in the DSC lattice, the secondary dislocation network can be formed by dislocations with Burgers vectors out of the crystal lattices, although these Burgers vectors may not be the smallest possible ones. An example in stainless steel was discussed by Bollmann, Michaut & Sainfort (1972). The fact that crystal dislocations can act as secondary dislocations seems to be related to the low stacking-fault energy of stainless steel.

3.2.2. *The conservation of a crystallographic axis*

Now, the case is discussed which actually started this whole research on continuous dislocation distributions. It is the problem of a relative orientation such that a crystallographic axis is nearly common to both crystals but that the relaxation pattern for the closest rotation on the crystallographic axis is not periodic. It is the case which corresponds to the 'plane matching' model of Pumphrey (1972). Warrington & Boon (1975) have calculated the probabilities for relative orientations of the two crystal lattices falling into a range where a common, low-index crystallographic axis could be conserved.

In order to fix our ideas, let us assume a rotation of $\theta=20°$ around the [001] axis in the primitive cubic (p.c.) structure. This orientation is relatively far from $\Sigma=25$, ($\theta=16{\cdot}26°$, [001]) and $\Sigma=13$ ($\theta=22{\cdot}62°$ [001]). The DSC lattices of the two coincidence orientations are 'layer structures' with layers in the (001) planes spaced by a[001]. The layers contain a discrete finer

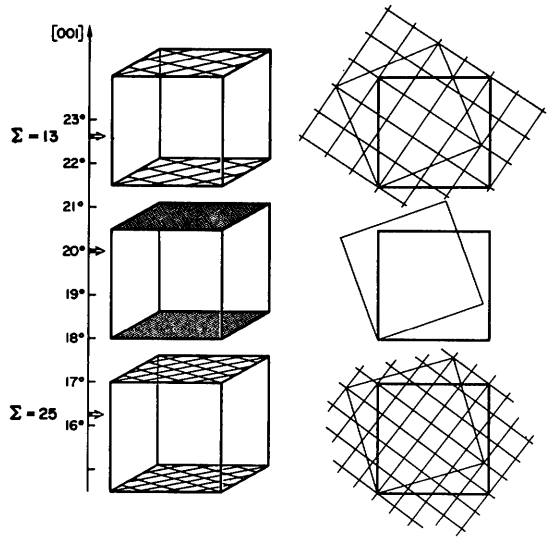


Fig. 4. DSC-lattices for the p.c. structure for $\Sigma=25$, $\theta=16{\cdot}26°$ and $\Sigma=13$, $\theta=22{\cdot}62°$ and in between the semicontinuous DSC lattice for $\theta=20°$. The cube represents the unit cell of the crystal lattice.

two-dimensional lattice of points (Fig. 4). Any rotation on the [001] axis can be arbitrarily close to a 'rational' rotation [tan $(\theta/2)$ = rational number]. Large Σ values, however, may loose their physical significance since the crystal may not be able to distinguish energetically between a periodic pattern with a large period and one which is not periodic at all. The 20° rotation is, for example, close to $\Sigma=125$ (which means that the period of the pattern contains 125 crystal units) and close to $\Sigma=149$. Hence, in the case of the conservation of the common crystallographic axis [001] alone, the DSC lattice consists of continuous (001) layers spaced by the lattice constant a. Continuous layers would indicate the presence of 'continuous' dislocation distribution.

The problem of the present research was to investigate the meaning of these continuous dislocations. More specifically we ask in the case of a rotation of $\theta°$ in the crystallographic axis combined with a rotation of $\vartheta°$ perpendicular to that axis for the difference in the relaxation pattern between the state where the axis is conserved and that where it is not conserved, or concretely: how can these two states be distinguished in an electron micrograph for example?

We describe the solution along two parallel lines. On the first line we determine the O lattice of the total rotation $\mathbf{R}(\theta_t)=\mathbf{R}(\vartheta)\mathbf{R}(\theta)$, which furnishes the answer in the case where the θ axis is not conserved. The second line is that with the semicontinuous DSC lattice, which furnishes the result when the θ axis is conserved.

If the axis of the rotation is not perpendicular to a crystallographic plane which contains a flat b net composed of possible Burgers vectors [*e.g.* the (001) or (111) plane in the f.c.c. structure], the b net, which has to approximate the b subspace (here the plane perpendicular to the rotation axis), becomes stepped. The steps in the b net represent an additional set of dislocations which we call 'b-step dislocations'*). We discuss first these b-step dislocations (Fig. 5).

b-step dislocations

First line. With $\mathbf{R}(\theta)$ in the [001] axis and $\mathbf{R}(\vartheta)$ in the [100] axis, the angle θ_t of the total rotation $\mathbf{R}(\vartheta)\mathbf{R}(\theta)$ is given by:

$$\cos(\theta_t/2)=\cos(\theta/2)\cos(\vartheta/2), \tag{3.3}$$

and the rotation axis by

$$[\text{cotan}(\theta/2), -1, \text{cotan}(\vartheta/2)] \tag{3.4}$$

which means that the angle between the x axis and the rotation axis projected on the xy plane is $-(\theta/2)$ and correspondingly in the yz plane with respect to the z axis, $-(\vartheta/2)$.

The plane perpendicular to this axis through the coordinate origin is the b subspace. This inclined plane of the b subspace has to be intersected by the horizontal layers of the b lattice (which looks the same as the crystal lattice 1). The intersecting lines have to be transformed by $[\mathbf{I}-\mathbf{R}^{-1}(\theta_t)]^{-1}$ which is a rotation by $[(\theta_t/2)-(\pi/2)]$ around the rotation axis of the total rotation and an expansion by

$$\left[(\tfrac{1}{2})^2\,\text{cotan}^2\left(\frac{\theta_t}{2}\right)+(\tfrac{1}{2})^2\right]^{1/2}=\frac{1}{2\sin(\theta_t/2)}. \tag{3.5}$$

The lines so obtained, together with the rotation axis, determine a set of parallel O planes, The intersection of the cell walls (intermediate planes between the O planes) with the grain boundary are the b-step dislocations. In our example the central O plane passes through the x axis and is inclined by $(\vartheta/2)$ away from the z axis towards the negative y axis (Fig. 6).

Second line. On the second line with the semicontinuous DSC lattice, exactly the same procedure can be followed, only that here the axis of rotation is the [100] axis of the $R(\vartheta)$ rotation, and the rotation angle is ϑ instead of θ_t. The result is the same as in the first case (Fig. 7). [It is also the same for both cases (but different from the above example) if the ϑ axis has an

* In (I), p. 129, these were called 'foreign dislocations'. That notation, however, is somewhat confusing and vague since the b-step dislocations are intrinsic to the boundary and not foreign to it.

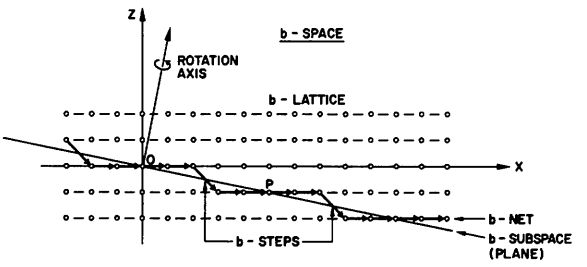


Fig. 5. Notation for different features in the b space.

arbitrary orientation in space.] The b-step dislocations are visible in electron micrographs as sets of parallel lines in the boundary.

Hence, the existence of the b-step dislocations does not tell whether a common crystallographic axis is conserved. It shows only that the rotation axis is close to a low index crystallographic axis. (*i.e.* an axis perpendicular to a flat b net). Energetically it is expected that these additional b-step dislocations will anyhow increase the boundary energy compared to a rotation exactly in the crystallographic axis, whether the common axis is conserved or not. Now we discuss the details of the relaxation pattern apart from the b-step dislocations.

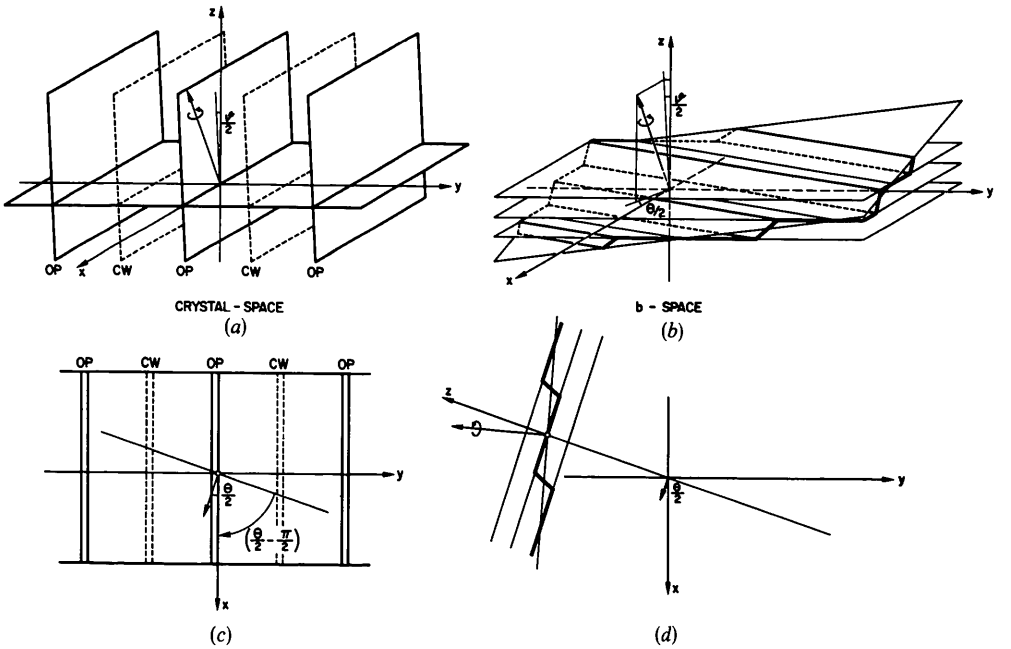


Fig. 6. Determination of the b-step dislocations starting from the total rotation. (OP = O plane, CW = cell wall). The intersections of the grain boundary with the cell walls are the dislocations. (*a*) Perspective view in crystal space. (*b*) Top view in crystal space. (*c*) Perspective view in b space. (*d*) Top and front view in b space.

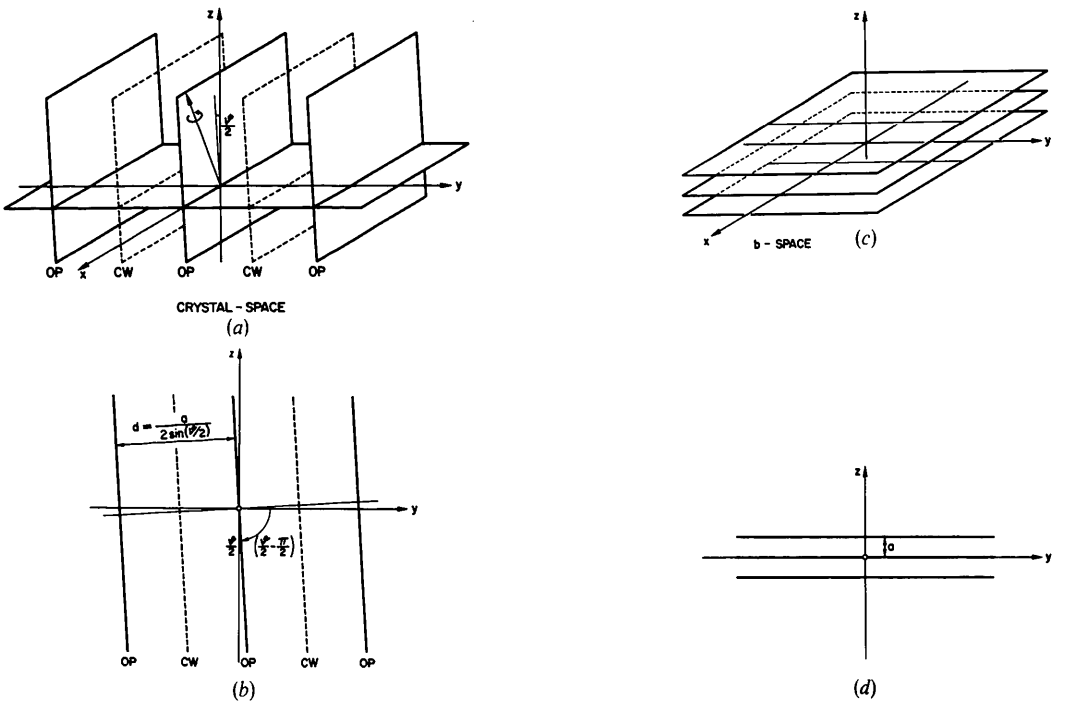


Fig. 7. Determination of the b-step dislocations starting from the DSC lattice. Here, the rotation axis is the x axis. (See caption of Fig. 6.)

Relaxation pattern

First line. The total O lattice is calculated by the standard procedure for the primary dislocation network. The b lattice points of the b net are projected* on the b subspace, then transformed by $[\mathbf{I}-\mathbf{R}(\theta_t)^{-1}]^{-1}$, and through the resulting points in the b subspace, the O lines are placed in the direction of the inclined axis θ_t. The O-lattice cell structure is then a tube structure in the direction of the rotation axis, sectioned by the planes of the b-step dislocations. A boundary placed perpendicularly to the rotation axis (tube axis) is, roughly speaking, a superposition of a twist (θ) and a tilt (ϑ) boundary.

Second line. Here we have to follow the O-lattice procedure with the semicontinuous DSC lattice. The DSC lattice seen as a b lattice means that the Burgers vectors in the continuous layers are continuous, while out of them they are discrete. In the p.c. structure the discrete Burgers vectors are of the [001] type. The b secondary subspace is, in our example, the (100) plane. Here the O lattice tube structure lies in the [100] direction. The continuous DSC lattice can be considered as the limiting case of a discrete lattice and so can the O lattice (Fig. 8). If the boundary is placed passing through the [100] axis, but otherwise in an arbitrary orientation, it must contain ledges. Between the ledges the primary O lattice is a tube structure parallel to the z axis corresponding to the θ rotation.

These ledges are the answer to our question concerning the difference between the conserved or not-conserved axis. If the axis is not conserved, a corresponding boundary can be smooth. In the first case the virtual continuous dislocations representing the displacement field of the difference rotation are continuously distributed, in the second case they are not grouped into discrete dislocations anymore, but aligned on the walls of the ledges which are located between the b-step dislocations.

Hence, a discrete b lattice or DSC lattice means grouping of the continuous dislocations to form discrete dislocations, a semicontinuous DSC lattice means an alignment of the continuous dislocation on ledges. Whether this kind of relaxation is actually energetically preferred has to be decided from observations.

* In the comparison between the two states: 'crystallographic axis conserved or not' it has proved to be crucial that the b lattice points are projected into the b subspace in the direction of the conserved axis, which in our case is not perpendicular to the b subspace.

Summary

The link between the continuous displacement field in the interface between two bodies which are related by a homogeneous linear transformation, and the discrete dislocation network between two correspondingly joined crystals, is given by the possibility of representing any such displacement field in an infinite number of ways by continuous distributions of dislocations. The discrete dislocations can then be understood as bundles of continuous dislocations. The specific continuous dislocation distribution and its grouping into discrete dislocations is governed by conservation principles. These principles are, on the primary level, the local conservation of the crystal structure and, on the secondary level, the local conservation of an energetically preferred relaxation pattern.

The O-lattice theory is discussed in relation to the continuous dislocation distributions for the primary and the secondary level. The aspect of the O-lattice theory has changed insofar as before it was thought that the crystals either conserve locally the crystal structure or at least a common substructure (coincidence site lattice, common axis). Now the 'either/or' has changed to an 'as well as'. The primary condition of the local conservation of the crystal structure is considered to govern any state, while the secondary level appears occasionally in addition to the primary one.

A special problem is a state where the relative orientation of the two crystal lattices is such that they have nearly a low index crystallographic axis in common,

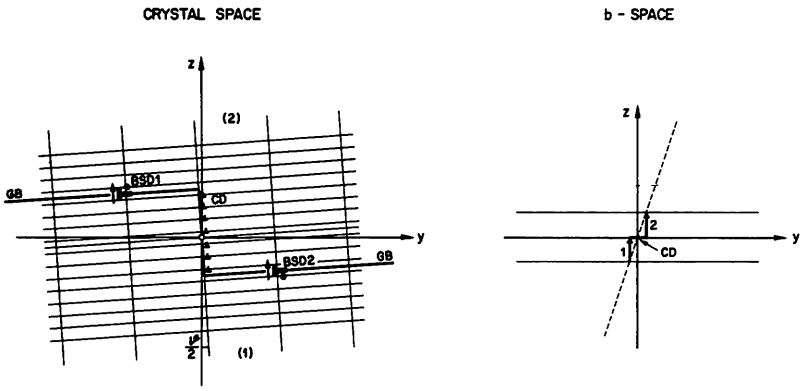


Fig. 8. Configuration of the grain boundary (GB) when a common crystallographic axis is conserved. (BSD = b-step dislocation, CD = continuous dislocation). The continuous dislocations are aligned on ledges.

but that the closest state with the common axis is no coincidence state (no periodic relaxation pattern). It is shown that, if the state of the common axis is not preferred, the boundary is expected to be smooth while in the case of the conserved axis, a boundary in a general orientation is expected to show ledges, where in one type, ledge-walls, the continuous dislocations are aligned, but not grouped to form discrete dislocations.

Although the theorem has been treated in a formal mathematical way there may be some physical significance involved. The dislocation network (primary and secondary) in the boundary is determined by the energetically favorable feature to be conserved. This feature, however, may change, for example, with temperature, so that at low temperatures a relatively high Σ value of a coincidence orientation may be conserved while at higher temperatures it may no longer be favoured. At that moment the discrete secondary dislocation network would spread out and eventually form another dislocation network related to another neighbouring Σ value (Gleiter, 1976). Similar events may happen in a boundary on a phase change or in recrystallization (Balluffi, 1976). Our theorem may help to obtain a better quantitative understanding of such changes.

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APPENDIX *A*

Decomposition of a rotation field into two sets of continuous dislocations

The problem is treated two-dimensionally. We assume a structure given by the following structure matrix (the column vectors of which are the unit vectors of crystal 1, in orthonormal coordinates) (for $\psi = 30°$ see Fig. 3):

$$\mathbf{S} = \left(\begin{array}{c|c} 1 & -\sin\psi \\ 0 & \cos\psi \end{array}\right) = \mathbf{B}^{(L)}. \tag{A1}$$

$\psi = 0$ represents the p.c. structure.

The O lattice then becomes:

$$\mathbf{X}^{(0)} = [\mathbf{I} - \mathbf{R}(\theta)^{-1}]^{-1}\mathbf{B}^{(L)} = \mathbf{T}^{-1}\mathbf{B}^{(L)} \tag{A2}$$

with $\mathbf{T}^{-1}$ from (3.1)

$$\mathbf{X}^{(0)} = \left(\begin{array}{c|c} \frac{1}{2} & -\frac{1}{2}\sin\psi + \frac{1}{2}\operatorname{cotan}\left(\frac{\theta}{2}\right)\cos\psi \\ -\frac{1}{2}\operatorname{cotan}\left(\frac{\theta}{2}\right) & \frac{1}{2}\operatorname{cotan}\left(\frac{\theta}{2}\right)\sin\psi + \frac{1}{2}\cos\psi \end{array}\right). \tag{A3}$$

The neutral lines of the shear transformations are now placed into these O-lattice unit vectors. Unit vectors perpendicular to these vectors are the normal on the shear planes. They are represented as row vectors in the matrix $\mathbf{N}$

$$\mathbf{N} = \begin{pmatrix} \sin\left(\frac{\theta}{2}+\psi\right) & -\cos\left(\frac{\theta}{2}+\psi\right) \\ \cos\left(\frac{\theta}{2}\right) & \sin\left(\frac{\theta}{2}\right) \end{pmatrix}. \tag{A4}$$

The displacement field of the rotation is

$$\mathbf{T} = [\mathbf{I} - \mathbf{R}^{-1}(\theta)] = \begin{pmatrix} 1-\cos\theta & -\sin\theta \\ \sin\theta & 1-\cos\theta \end{pmatrix}$$

$$= 2\sin\left(\frac{\theta}{2}\right)\begin{pmatrix} \sin\left(\frac{\theta}{2}\right) & -\cos\left(\frac{\theta}{2}\right) \\ \cos\left(\frac{\theta}{2}\right) & \sin\left(\frac{\theta}{2}\right) \end{pmatrix}. \tag{A5}$$

According to (2.13)

$$\mathbf{WN} = \mathbf{T} \tag{A6}$$

or

$$\mathbf{W} = \mathbf{TN}^{-1}; \tag{A7}$$

it follows that:

$$\mathbf{W} = \left(\begin{array}{c|c} 2\sin\left(\frac{\theta}{2}\right) & -2\sin\left(\frac{\theta}{2}\right)\tan\psi \\ \hline \cos\psi & \\ 0 & 2\sin\left(\frac{\theta}{2}\right) \end{array}\right). \tag{A8}$$

Now the two shear fields are given by:

$$(\mathbf{I} - \mathbf{H}_1^{-1}) = \left(\begin{bmatrix} 2\sin^2(\theta/2) \\ +\sin\theta\tan\psi \\ 0 \end{bmatrix}\begin{bmatrix} -\sin\theta \\ +2\sin^2(\theta/2)\tan\psi \\ 0 \end{bmatrix}\right) \tag{A9}$$

$$(\mathbf{I} - \mathbf{H}_2^{-1}) = \begin{pmatrix} -\sin\theta\tan\psi & -2\sin^2\left(\frac{\theta}{2}\right)\tan\psi \\ \sin\theta & 2\sin^2\left(\frac{\theta}{2}\right) \end{pmatrix} \tag{A10}$$

which obviously sum to the rotation field (*A*5).

The grouping procedure and the attribution of the Burgers vectors is shown in Fig. 3 for $\psi = 30°$.

APPENDIX *B*

The relaxation pattern as determined by the *O*-lattice method

The O-lattice theory is a purely geometrical procedure. Hence, it is not to be expected to obtain a fully realistic picture of the atomic arrangement in the boundary. This theory is a kind of a 'crystallography' of the boundary, it furnishes an 'ideal' boundary which is

thought to be a reference system to a real boundary, like an ideal crystal is a reference system to the real crystal. Starting from an ideal model of a boundary, which, however, has to be close enough to the real arrangement, new concepts, such as, for example, boundary defects can be formulated.

As an example, we show a tilt boundary in the $\Sigma=25$ case of the p.c. structure ($\theta=16{\cdot}26°$, [001]). We consider the two crystal lattices (without atoms) as interpenetrating and determine the O lattice cell structure, Fig. 9. Every O point is an origin onwards from which the closest neighbour points in both lattices are related by the 16·26° rotation. We connect the two neighbour points by a bar. Hence, every bar has a lattice 1 and a lattice 2 end. A bar represents the position of a single atom.

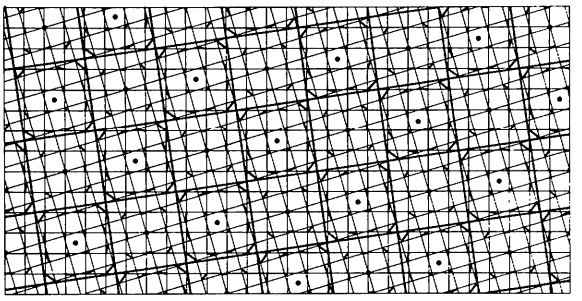
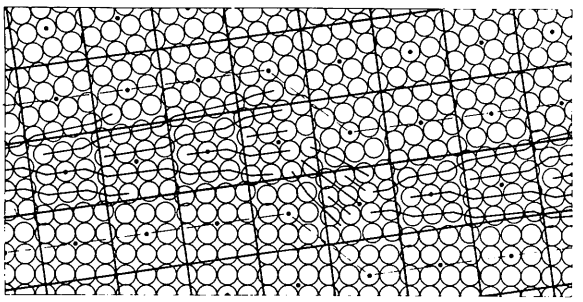


Fig. 9. O-lattice of the primitive cubic structure ($\Sigma=25$, $\theta=16{\cdot}26°$, [001]-axis). The closest neighbour points in the two lattices are connected by a bar.



(*a*)

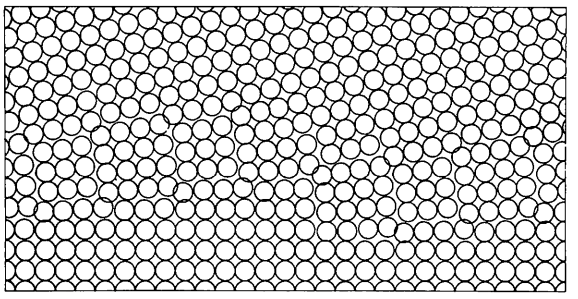


Fig. 10. (*a*) Stepped tilt boundary in the O lattice of Fig. 9. The dislocations appear at the cell walls. (*b*) Same boundary as in (*a*).

Now, we decide on the path of the boundary through O elements and determine a boundary zone of one O lattice unit width to both sides. The atoms are then placed, on the crystal 1 side of the boundary up to the limit of the boundary zone, exactly into the lattice 1 positions, and accordingly on the crystal 2 side.

In the boundary zone the atoms are placed on the bar according to

$$x=x^{(1)}+\lambda[x^{(2)}-x^{(1)}] \qquad (B1)$$

where λ varies linearly with the position of the centre of the bar within the boundary zone ($\lambda=0$ at the crystal 1 zone limit, $\lambda=0{\cdot}5$ on the boundary plane and $\lambda=1$ at the crystal 2 zone limit). The result is shown in Fig. 10(*a*). The dislocations appear automatically at the O-lattice cell walls and the Burgers vectors are those which are attributed by the duality relations. The coincidence sites are positions belonging to lattice 1 as well as to lattice 2 when extrapolated from both sides of the boundary zone. Fig. 10(*b*) shows the same picture without the reference frame. This procedure can also be applied for a twist boundary perpendicular to the O lines or any other boundary orientation by choosing the width of the boundary zone appropriately.

This linear model has the following properties. (1) It can be constructed for any boundary. (2) It has exactly the density of the perfect crystal (which may not be realistic). However, the atoms do not excessively overlap nor do they leave large holes. (3) The linear dependence of λ and the straight boundary zone limit may not be fully realistic either.

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