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Recurrence properties of *O*-lattices and the classification of grain boundaries

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A recurrence relation is shown to exist between *O*-lattices of rotation-related grain boundaries (GBs) when a suitable parametrization of the rotation angle is introduced. This relation allows the basis vectors of any *O*-lattice to be calculated by a simple vector addition if the basis vectors of any two orientations are known. Its main usefulness, however, lies in the fact that it induces a partition of the angular space into disjoint sets, which groups grain boundaries into a finite number of equivalence classes, each represented by a special singular boundary (normal form). This shows that the *O*-lattice theory contains within it a much sought after general classification scheme for interfaces independent of the crystal system and therefore completely general.

1. Introduction

Perhaps the most important goal in the grain-boundary (GB) field is to find a general theory able to relate the physical properties to the atomic structure. One problem has been the difficulty in finding a general (system-independent) theory capable of providing structural information as a function of measurable external parameters such as the crystallographic structure and relative orientation of the parent grains. One theory that deserves special mention is Bollmann's *O*-lattice theory (Bollmann, 1970), which provides the dislocation content of arbitrary interfaces. Bollmann's theory is completely derived from first principles, sustained by a solid mathematical foundation and completely general. Its main drawback, however, is that it does not provide a detailed (atomistic) picture of the interface. In the hope of determining the detailed structure of GBs, a common course of action has been to classify GBs into property-related classes such as symmetry (Pond & Bollmann, 1979; Pond & Vachlavas, 1983) and structural units configuration (Sutton & Vitek, 1980). However, in spite of these efforts, in practice GBs are still crudely classified into three main groups: low angle, special or singular and general.

The purpose of this paper is to show that if the rotation angle is properly parameterized then a recurrence relation between *O*-lattices of rotation-related GBs emerges. The parametrization induces a partition of the angular space into an effectively finite number of disjoint angular intervals. The recurrence relation links the *O*-lattices of GB lying in adjacent intervals. The partition of the angular range into disjoint intervals actually groups GBs into equivalence classes; all GBs contained within a given interval belong to a class that shares structural features. This means that the *O*-lattice theory alone produces a classification of GBs that is independent of the crystal system and is therefore completely general. In this scenario, each equivalence class is associated with a special GB (or normal form), which is a special (singular) boundary in the sense that it contains only primary dislocations and has a particularly simple structure.

2. Angular parametrization

Consider two lattices L_1 and L_2 such that $L_2 = \mathbf{R}L_1$, with $\mathbf{R}$ denoting a rotation through an angle θ around a given crystallographic axis $\langle hkl\rangle$. For any rotation angle θ between L_1 and L_2, we can always write (Romeu, 2003)

$$\tan(\theta/2) = N^{1/2}\xi^{-1}, \tag{1}$$

where $N = h^2 + k^2 + l^2$ and ξ is a real number. As we shall see, the above parametrization has important consequences, but for the time being notice that it is useful in that it allows the separation of the axis and angle contributions into the variables N and ξ. If we define x as the closest integer to ξ and $\delta = \xi - x$ as the fractional part of ξ contained in the interval $(-\frac{1}{2}, \frac{1}{2})$, then

$$\xi = x + \delta \tag{2}$$

and equation (1) becomes

$$\tan(\theta/2) = N^{1/2}\frac{1}{\xi} = N^{1/2}\frac{1}{x+\delta}. \tag{3}$$

If we restrict δ to take on only rational values then the previous equation reduces to the well known Ranganathan equation $\tan(\theta/2) = N^{1/2}p/q$, where $N = |\langle hkl\rangle|^2$ and p, q are integers (Ranganathan, 1966) giving the possible angles between rotation-related coincidence boundaries in the cubic system. It must be noted that, owing to symmetry considerations, different integers p, q in Ranganathan's equation may yield the same structure. For example, for rotations around $\langle 001\rangle$, $N = 1$ and $\theta = 2\tan^{-1}(p/q)$ but, since any rotation by 90° leaves the structure unchanged, the same structure is obtained for $(q-p)/(q+p)$, $(q+p)/(q-p)$ and q/p, corresponding to the angles $90° - \theta$, $90° + \theta$ and $180° - \theta$. In general, if the rotation angle is restricted to the interval $[0, \alpha/2]$ with α = symmetry angle of the rotation axis, then the quotient p/q is uniquely determined.

Note that, while Ranganathan's equation is valid only for the cubic case, the above parametrization is valid always. If additionally ξ is an integer ($\delta = 0$), then the resulting interface is a singular coincidence boundary that contains only primary dislocations. Conversely, if $\delta \neq 0$, then the interface contains secondary dislocations whose spacing is a function of δ (Romeu, 2003).

If θ is small, $x + \delta$ is a large number and its fractional part δ can be neglected. Hence, although small-angle boundaries are indeed singular boundaries (recall they are composed of primary dislocations), they are so close together ($\delta \ll x$) that it is no longer justifiable

to call them singular and they form a class of their own. As a result, although the number of singular boundaries (angular intervals) is actually infinite, only a finite number of them need be considered.

3. The *O*-lattice in two dimensions

In the coordinate system of L_1, the inverse of the displacement field matrix $T = (I - R^{-1})$ is given by

$$T^{-1} = \frac{1}{2N^{1/2}} \begin{pmatrix} N^{1/2} & \xi \\ -\xi & N^{1/2} \end{pmatrix}. \quad (4)$$

According to Bollmann, if $\mathbf{A}$ is the structure matrix of the L_1 lattice, then a basis for the *O*-lattice is given by the columns of the structure matrix $\mathbf{O}$ given by

$$\mathbf{O} = T^{-1}\mathbf{A}. \quad (5)$$

It is easy to see from equation (4) that T^{-1} can also be written as

$$T^{-1} \equiv T_\xi^{-1} = \tfrac{1}{2}I + \xi \frac{1}{2N^{1/2}} R_{-\pi/2} \quad (6)$$

with I and $R_{-\pi/2}$ being the identity matrix and a rotation through $-\pi/2$. In order to simplify notation, we write

$$R_N = \frac{1}{2N^{1/2}} R_{-\pi/2} \quad (7)$$

so that equation (3) becomes

$$T_\xi^{-1} = \tfrac{1}{2}I + \xi R_N. \quad (8)$$

The usefulness of equation (8) lies in the fact that the angle and rotation-axis contributions to the *O*-lattice have been explicitly separated into the terms ξ and R_N. With this we now can write T_ξ^{-1} in terms of x and δ as

$$T_\xi^{-1} = T_x^{-1} + \delta R_N \quad (9)$$

so that the *O*-lattice is given by

$$\mathbf{O}_\xi = T_\xi^{-1}\mathbf{A} = T_x^{-1}\mathbf{A} + \delta R_N \mathbf{A}, \quad (10)$$

or more clearly

$$\mathbf{O}_\xi = \mathbf{O}_x + \delta R_N \mathbf{A}. \quad (11)$$

Therefore, if the *O*-lattice $\mathbf{O}_x$ for a singular orientation x is known, then all *O*-lattices within the interval $(x - \frac{1}{2}, x + \frac{1}{2})$ can be readily calculated by adding $\delta R_N \mathbf{A}$, whose columns, according to equation (7), are the basis vectors of L_1 rotated by $-\pi/2$ and scaled by $\delta/(2N^{1/2})$.

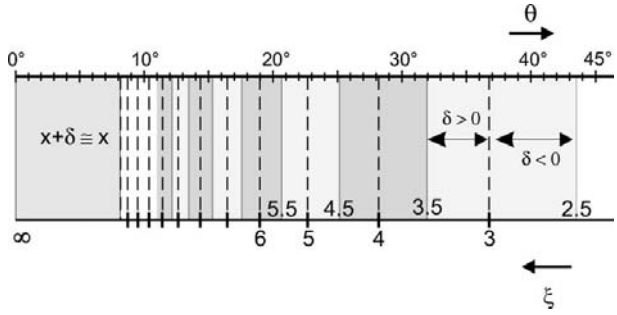

Figure 1
Angular range for [001] twist GBs labelled using degrees and the dimensionless parameter ξ. Adjacent intervals have been highlighted using alternating shades of grey. Note that, for small θ, $x \gg \delta$, the intervals become arbitrarily small ($\xi \simeq x$) so that all small-angle GBs are singular. As a result, small-angle GBs belong to a class of their own.

Note that equation (11) effectively partitions the angular space into intervals of length $\Delta\xi = 1$ centred on the integer x which can be used to label the interval. The real number δ then defines the position of a GB within a given interval. All GBs that share the same interval position, *i.e.* the same value of δ, are related [see equation (13)].

4. Recurrence relation between *O*-lattices

Using equation (9), it follows that, for a given rotation axis,

$$T_\xi^{-1} - T_{\xi-1}^{-1} = T_x^{-1} - T_{x-1}^{-1} = R_N$$

and

$$\mathbf{O}_\xi - \mathbf{O}_{\xi-1} = \mathbf{O}_x - \mathbf{O}_{x-1} = R_N\mathbf{A}. \quad (12)$$

The last equation implies that, for a given rotation axis, the basis vectors of two *O*-lattices differing in angular parameter by one are related by the columns of the matrix $R_N\mathbf{A}$, which is a constant for a given rotation axis [see equation (7)].

Using equations (11) and (12), it follows that

$$\mathbf{O}_\xi = \mathbf{O}_x + \delta(\mathbf{O}_x - \mathbf{O}_{x-1}).$$

In particular, if $\delta = 1$ then $O_\xi = O_{x+1}$ and we obtain the recurrence relation:

$$\mathbf{O}_{x+1} = 2\mathbf{O}_x - \mathbf{O}_{x-1}.$$

More generally, since by equation (12) $\mathbf{O}_\xi - \mathbf{O}_{\xi-1} = \mathbf{O}_{\xi+1} - \mathbf{O}_\xi$, it follows that

$$\mathbf{O}_{\xi+1} = 2\mathbf{O}_\xi - \mathbf{O}_{\xi-1}. \quad (13)$$

Take the example of (001)-rotation GBs in the cubic system and suppose the *O*-lattices of two particularly simple systems are known such as $\Sigma = 1$ ($\theta = 90°$, $x = 1$) and $\Sigma = 5$ ($\theta = 53.1°$, $x = 2$). Using equation (11), all *O*-lattices in the equivalence classes $x = 1$ and $x = 2$ are known. Then using equation (13) all *O*-lattices in the angular range can be calculated. See Fig. 1.

5. Conclusions

In this work, we have shown that, when the angle between two identical lattices is properly parameterized, the angular range becomes naturally partitioned into disjoint intervals which group GBs into equivalence classes. It has been shown elsewhere (Romeu, 2003) that all GBs in a given class have common structural features that can be deduced from the structure of the singular normal form located at the centre of the parameterized intervals $[x_i \pm \frac{1}{2}]$, where the angular parameter $\xi = x$ is an integer. We have also shown that there is a recurrence relationship that relates the *O*-lattices of GBs contained in adjacent intervals (classes), so that knowing the *O*-lattice for two orientations around a given crystallographic axis suffices to calculate the *O*-lattice for any orientation.

References

Bollmann, W. (1970). *Crystal Defects and Crystalline Interfaces.* Berlin: Springer.
Pond, R. C. & Bollmann, W. (1979). *Philos. Trans. R. Soc. London Ser. A*, **292**, 449–472.
Pond, R. C. & Vlachavas, D. S. (1983). *Proc. R. Soc. London Ser. A*, **386**, 95–143.
Ranganathan, S. (1966). *Acta Cryst.* **21**, 197–199.
Romeu, D. (2003). *Phys. Rev. B*, **67**, 024202.
Sutton, A. P. & Vitek, V. (1980). *Scr. Metall.* **14**, 129–132.