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Conditions for Singularity of Twist Grain Boundaries between Arbitrary 2-D Lattices

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ABSTRACT

We have shown that the expression $\theta = 2\tan^{-1}\sqrt{N}/\xi$ derived by Ranganathan to calculate the angles at which there exists a CSL for rotational interfaces in the cubic system can also be applied to general (oblique) two-dimensional lattices provided that the quantities σ^2 and $\sigma/\cos(\alpha)$ are rational numbers, with $\sigma = |\boldsymbol{b}|/|\boldsymbol{a}|$ and α is the angle between the basis vectors ***a*** and ***b***. In contrast with Ranganathan's results, *N*; given by $N = \tan^2(\alpha)$ needs no longer be an integer. Specifically, vectors ***a*** and ***b*** must have the form $\boldsymbol{a} = (1,0)$; $\boldsymbol{b} = (r, \tan\alpha)$ where r is an arbitrary rational number. We have also shown that the interfacial classification of cubic twist interfaces based on the recurrence properties of the O-lattice remains valid for arbitrary two-dimensional interfaces provided the above requirements on the lattice are met.

Keywords: Grain Boundaries; Crystallography of Interfaces; Coincidence Site Lattice

1. Introduction

In a now classic paper Ranganathan [1] showed that a Coincidence Site Lattice exists between two rotated cubic lattices when the rotation angle can be expressed as [1]

$$\tan\left(\frac{\theta}{2}\right) = \frac{y\sqrt{N}}{x} \tag{1}$$

where *x*, *y* are coprime integers and $N = h^2 + k^2 + l^2$ is an integer equal to the square of the magnitude of the crystallographic rotation axis $\boldsymbol{c} = [hkl]$. He also provided a procedure to find the index number Σ (the quotient between the areas of the unit cells of the CSL and the cubic lattices) as a function of *N*, *x* and *y*. In this paper we show that this equation is also valid for arbitrary (oblique) two dimensional lattices provided their basis vectors fulfill certain rationality conditions. Specifically, we will show that a two-dimensional CSL exists when the rotation angle θ given by

$$\theta = 2\tan^{-1}\frac{\sqrt{N}}{\xi} \tag{2}$$

where *N* is a real number that depends only on the lattice and ξ is a rational number. Reducing the problem to two dimensions makes the generalization to arbitrary twist grain boundaries tractable while it is not in itself major shortcoming since twist interfaces are two dimensional systems.

Besides its mathematical novelty, this result makes it possible to extend to arbitrary lattices a recent classification scheme for cubic GBs [2] based on the recurrence properties of the O-lattice [3] in combination with the angular parameterization introduced by Equation (2). In this scheme the angular space is partitioned into disjoint intervals $\xi \in [x - 1/2, x + 1/2)$ centered around every integer *x*. This partitioning groups GBs into an effectively finite number of equivalence classes [2], each containing a special (singular) interface which is the normal form of the class. Normal forms have the property of having a particularly simple structure [4,5] composed of structural elements (translational states) [4] also presented in all the elements of each class (see Section 5). Singular interfaces are located at the centre of each interval at the angles θ_x obtained by inserting integral values of ξ into Equation (2). The classification of interfaces is important since it allows, in principle, the description of physical properties in terms of differences and/or similarities with ideal defect-free structures akin to the crystalline Bravais lattices. Other work in this direction includes classification efforts based on symmetry variants [6,7] and structural units [8,9]. Without a crystallography of interfaces it is difficult to tell whether a given property is specific of a particular interface or shared by a whole collection of them.

In the following sections we review Ranganathan's approach towards the derivation of Equation (1), we then extend it to two dimensional interfaces to calculate the explicit form that the basis vectors of 2D lattices must have. Finally we show an example of a rhombic lattice showing that an interface in the class x has common elements with the normal form of the class.

2. Ranganathan's Method

In this section we extend Ranganathan's approach to two-dimensional lattices that are not planes of a cubic lattice. We will see that Ranganathan's approach still gives coincidences but some rationality conditions must be imposed on the lattices. Also, N is not any longer related to any crystallographic direction but depends exclusively on the nature of the lattice.

In what follows we shall use $\boldsymbol{L}$ to indistinctly refer to a lattice and its structure matrix. Let $\boldsymbol{L}$ a cubic lattice in ordinary three-dimensional space and assume $\boldsymbol{L}_2 = R\boldsymbol{L}$ where R is a rotation through the angle θ around the crystallographic axis $[hkl]$. We want to know when such a rotation leads to coincidences; in other words, when is $\boldsymbol{L}_2 \cap \boldsymbol{L} \neq \{\boldsymbol{0}\}$.

The strategy followed by Ranganathan [1] involved first asking when the (hkl) plane of a cubic crystal contains a rectangular sublattice. He noticed that the answer is always in the affirmative: the orthogonal vectors $\boldsymbol{a} = \begin{bmatrix} 0 & l & \bar{k} \end{bmatrix}$ and $\boldsymbol{b} = \begin{bmatrix} \overline{k^2 + l^2} & hk & hl \end{bmatrix}$ are always on the (hkl) plane.

But a rectangular cell is always symmetric under a reflection with respect to one side of the rectangle. Then, for any vector $\boldsymbol{P} = x\boldsymbol{a} + y\boldsymbol{b}$ with x and y integers (which lies in $\boldsymbol{L}$) the vector $\boldsymbol{P}' = x\boldsymbol{a} - y\boldsymbol{b}$ (reflection with respect to the $\boldsymbol{a}$ side of the rectangle) is also in the lattice. Since the effect of this reflection is the same of a rotation through taking $\boldsymbol{P}$ into $\boldsymbol{P}'$ (see **Figure 1**), we conclude that such a rotation also brings the lattice into coincidence. The angle θ is given by

$$\tan\left(\frac{\theta}{2}\right) = \frac{y|\boldsymbol{b}|}{x|\boldsymbol{a}|} = \frac{y}{x}\sqrt{N}$$

with

$$N = |\boldsymbol{b}|^2 / |\boldsymbol{a}|^2 = h^2 + k^2 + l^2 \cdot$$

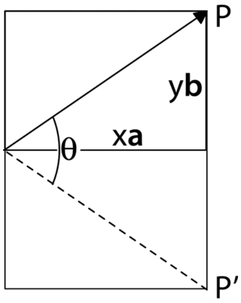

Figure 1. Ranganathan's rectangle. For any lattice vector *P* = *xa* + *yb* with x and y integers, the reflection with respect to the a side of the rectangle: *P′* = *xa* − *yb* is also in the lattice. The effect of this reflection is the same as that of a rotation through *θ*.

3. General Two-Dimensional Lattices

Following Ranganathan, we address here the problem of finding a rectangular cell that spans a sublattice of a general 2-D lattice. The lattice shall be referred to as $\boldsymbol{L}$ and we give a spanning set $\{\boldsymbol{a}, \boldsymbol{b}\}$.

The problem is to find two vectors $\boldsymbol{d}_1$, $\boldsymbol{d}_2 \in \boldsymbol{L}$ such that $\boldsymbol{d}_1 \cdot \boldsymbol{d}_2 = 0$. Then there must exist four integers u, v, x, y such that

$$\begin{aligned} \boldsymbol{d}_1 &= u\boldsymbol{a} + v\boldsymbol{b} \\ \boldsymbol{d}_2 &= x\boldsymbol{a} + y\boldsymbol{b} \\ \boldsymbol{d}_1 \cdot \boldsymbol{d}_2 &= 0 = (u\boldsymbol{a} + v\boldsymbol{b}) \cdot (x\boldsymbol{a} + y\boldsymbol{b}) \\ &= ux|\boldsymbol{a}|^2 + vy|\boldsymbol{b}|^2 + (uy + vx)(\boldsymbol{a} \cdot \boldsymbol{b}) \\ &= ux|\boldsymbol{a}|^2 + vy|\boldsymbol{b}|^2 + (uy + vx)|\boldsymbol{a}||\boldsymbol{b}|\cos\alpha \end{aligned}$$

where α is the angle between $\boldsymbol{a}$ and $\boldsymbol{b}$.

There are several cases to consider:

1) In the trivial case $\boldsymbol{a} \cdot \boldsymbol{b} = 0$, then $\boldsymbol{d}_1 = \boldsymbol{a}$ and $\boldsymbol{d}_2 = \boldsymbol{b}$.

2) The rhombic case $|\boldsymbol{a}| = |\boldsymbol{b}|$, in this case $(\boldsymbol{a} + \boldsymbol{b}) \cdot (\boldsymbol{a} - \boldsymbol{b}) = 0$ so $\boldsymbol{d}_1 = \boldsymbol{a} + \boldsymbol{b}$ and $\boldsymbol{d}_2 = \boldsymbol{a} - \boldsymbol{b}$.

3) In the most general case where $|\boldsymbol{a}| \neq |\boldsymbol{b}|$ and $\boldsymbol{a} \cdot \boldsymbol{b} \neq 0$. Here there is a solution with $v = 0$ (or $u = 0$) provided that

$$ux|\boldsymbol{a}|^2 + uy|\boldsymbol{a}||\boldsymbol{b}|\cos(\alpha) = 0$$

$$ux + uy(|\boldsymbol{b}|/|\boldsymbol{a}|)\cos(\alpha) = 0$$

$$(|\boldsymbol{b}|/|\boldsymbol{a}|)\cos(\alpha) = -\frac{x}{y}$$

and this holds if $(|\boldsymbol{b}|/|\boldsymbol{a}|)\cos(\alpha)$ is a rational number m/n with m and n integers. Solving for $m/n = -x/y$ we have $v = 0$, $u = 1$, $x = -m$ and $y = n$, and using Equation (3) we have $d_1 = \boldsymbol{a}$ and $d_2 = nb - ma$. Sometimes it is convenient to use a rectangle that is not the smallest (in area) possible. This is the choice

$$\boldsymbol{d}_1 = m\boldsymbol{a},\ \boldsymbol{d}_2 = n\boldsymbol{b} - m\boldsymbol{a} \tag{4}$$

(see **Figure 2**).

Swapping the roles of $\boldsymbol{a}$ and $\boldsymbol{b}$ we see that $\left(|\boldsymbol{b}|/|\boldsymbol{a}|\right)\cos(\alpha)$ must be also rational and, consequently, $|\boldsymbol{b}|^2/|\boldsymbol{a}|^2$.

In what follows we will work in this general setting, since the rectangular and rhombic cases are particular instances.

3.1. Finding Coincidences

Once we have a rectangular cell spanned by $\{\boldsymbol{d}_1,\boldsymbol{d}_2\}$ that generates a sublattice of $\boldsymbol{L}$, then by Ranganathan's argument it follows that there is a rotation that produces coincidences for every choice of integers x, y such that

$$\tan\left(\frac{\theta}{2}\right)=\frac{y|\boldsymbol{d}_2|}{x|\boldsymbol{d}_1|} \tag{5}$$

so if we call $\xi = y/x$ and $N=\left(|\boldsymbol{d}_2|/|\boldsymbol{d}_1|\right)^2$ we obtain

$$\tan\left(\frac{\theta}{2}\right)=\frac{\sqrt{N}}{\xi} \tag{6}$$

which is identical to Equation (2) except now N depends only on the lattice and does not have to be an integer, from Equation (4) it follows that N must be rational. Notice that $\sqrt{N}=\tan(\theta_1/2)$ where θ_1 is the angle for $\xi = 1$ so we can write

$$\tan\left(\frac{\theta}{2}\right)=\frac{1}{\xi}\tan\left(\frac{\theta_1}{2}\right) \tag{7}$$

For the second choice of rectangle $\boldsymbol{d}_1 = m\boldsymbol{a}$, $\boldsymbol{d}_2 = n\boldsymbol{b}-m\boldsymbol{a}$, we have $\boldsymbol{d}_1+\boldsymbol{d}_2 = n\boldsymbol{b}$, hence $\boldsymbol{d}_1$ and $\boldsymbol{d}_1+\boldsymbol{d}_2$ are parallel to $\boldsymbol{a}$ and $\boldsymbol{b}$ respectively so that the angle between $\boldsymbol{d}_1+\boldsymbol{d}_2$ and $\boldsymbol{d}_1$ is the same as the angle between $\boldsymbol{a}$ and $\boldsymbol{b}$. Using $\alpha=\theta_1/2$ we obtain

$$\tan\left(\frac{\theta}{2}\right)=\frac{1}{\xi}\tan\left(\frac{\alpha}{2}\right) \tag{8}$$

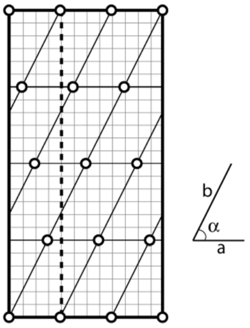

Figure 2. Two-dimensional lattice generated by the vectors (1,0) and (3/4, 6/4). Note the small rectangular cell with dashed vertical line is spanned by $\boldsymbol{d}_1$ = (1,0) and $\boldsymbol{d}_2$ = (0,4). The larger cell spanned by $\boldsymbol{d}_3$ = (3,0) and $\boldsymbol{d}_4$ = (0,4) has the property that the angle between $\boldsymbol{d}_3 + \boldsymbol{d}_4$ and $\boldsymbol{d}_3$ is the same as between *a* and *b*.

Notice that different choices of $\boldsymbol{d}_i$ will lead to the same set of angles θ because Equation (5) implies that given a rectangle $\boldsymbol{d}_1,\boldsymbol{d}_2$, if we choose a different one $\boldsymbol{d}_3 = h\boldsymbol{d}_1$, $\boldsymbol{d}_4 = k\boldsymbol{d}_2$ (for h, k integers or even rationals) the set

$$\left\{\tan\left(\frac{\theta}{2}\right)=\xi^{-1}\frac{|\boldsymbol{d}_4|}{|\boldsymbol{d}_3|}\right\}$$

is equal to the set

$$\left\{\tan\left(\frac{\theta}{2}\right)=\xi^{-1}\frac{|k||\boldsymbol{d}_2|}{|h||\boldsymbol{d}_1|}\right\}$$

the angles obtained for a given ξ are, however, different.

So far we have provided coincidences only along a line. Next we show that there is a genuine 2D CSL: consider the vector

$$\boldsymbol{P}^{\perp} = -yp\boldsymbol{d}_1 + xq\boldsymbol{d}_2$$

with x, y as before and p, q integers. This is a vector in the lattice and it is orthogonal to $\boldsymbol{P}=x\boldsymbol{d}_1+y\boldsymbol{d}_2$ if and only if p and q are chosen so as to satisfy

$$\frac{p}{q}=\frac{|\boldsymbol{d}_2|^2}{|\boldsymbol{d}_1|^2}=N$$

(they will be assumed to be coprime).

This shows that we can always construct a lattice vector orthogonal to $\boldsymbol{P}$ and it gives rise to another line of coincidences by exactly the same argument used to prove that $\boldsymbol{P}$ gives rise to a line of coincidences. Then a full two-dimensional CSL is ensured.

The area of the rectangle spanned by $\boldsymbol{P}$ and $\boldsymbol{P}^{\perp}$ is

$$A=|\boldsymbol{d}_1||\boldsymbol{d}_2|\left(x^2q^2+y^2p^2\right)$$

so

$$\frac{A}{|\boldsymbol{d}_1||\boldsymbol{d}_2|}=q^2\left(x^2+y^2N\right)$$

an expression that leads to Σ and agrees with the corresponding one in Ranganathan's work since in his case N is integer and, a fortiori, $q=1$.

4. Lattice Basis Vectors

Using elementary trigonometric identities it can be shown that the two-dimensional rotation matrix (with respect to a given orthonormal basis) and Equation (2) are given by

$$R=\begin{bmatrix}\cos(\theta) & -\sin(\theta)\\ \sin(\theta) & \cos(\theta)\end{bmatrix}=\frac{1}{\xi^2+N}\begin{bmatrix}\xi^2-N & -2\xi\sqrt{N}\\ 2\xi\sqrt{N} & \xi^2-N\end{bmatrix}$$

The lattice will be given by the basis $\boldsymbol{a}=(1,0)$ and $\boldsymbol{b}=\sigma(\cos\beta,\sin\beta)$; note we loose no generality by taking the first vector to be unitary. The structure matrix (the matrix having as columns the vectors of the lattice basis) is given by

$$\boldsymbol{L}=\begin{pmatrix}1 & \sigma\cos(\alpha)\\ 0 & \sigma\sin(\alpha)\end{pmatrix} \tag{9}$$

but, using Equations (6) and (8) and we get

$$\boldsymbol{L}=\begin{pmatrix}1 & \sigma\cos\alpha\\ 0 & \sigma\sqrt{N}\cos\alpha\end{pmatrix} \tag{10}$$

which equals

$$\boldsymbol{L}=\frac{\sigma}{\sqrt{1+N}}\begin{pmatrix}\dfrac{\sqrt{1+N}}{\sigma} & 1\\ 0 & \sqrt{N}\end{pmatrix} \tag{11}$$

or

$$\boldsymbol{L}=\begin{pmatrix}1 & \dfrac{\sigma}{\sqrt{N+1}}\\ 0 & \dfrac{\sigma}{\sqrt{N+1}}\sqrt{N}\end{pmatrix} \tag{12}$$

Consequently the rotation matrix with respect to the lattice basis (also known as transition matrix) is

$$T=\frac{1}{N+\xi^2}\begin{pmatrix}\xi^2-2\xi-N & -2\sigma^2\xi\dfrac{\sqrt{N+1}}{\sigma}\\ 2\xi\dfrac{\sqrt{N+1}}{\sigma} & \xi^2+2\xi-N\end{pmatrix}$$

which is a rational matrix (a necessary and sufficient condition for the existence of coincidences [10]) if ξ, N, σ^2 and

$$r=\frac{\sigma}{\sqrt{1+N}}=\sigma\cos\alpha \tag{14}$$

are rational numbers. Substituting r in Equation (12), the general form for the structure matrix $\boldsymbol{L}$ of an oblique lattice that can give rise to a CSL through rotations acquires the particularly simple form

$$\boldsymbol{L}=\begin{pmatrix}1 & r\\ 0 & r\sqrt{N}\end{pmatrix}=\begin{pmatrix}1 & r\\ 0 & r\tan\alpha\end{pmatrix} \tag{15}$$

which depends only on the angle α and size ratio σ of $\boldsymbol{a}$ to $\boldsymbol{b}$.

5. Singular vs Non-Singular Cases

Figure 3 illustrates that the parametrization of Equation (2) works for non cubic lattices. **Figure 3** shows an example of the difference in structure between a normal class interface and other interfaces in the class [2]. The figure shows the $\xi=5$ and $\xi=5+1/3$ interfaces for a lattice defined by the structure matrix which is of the form 12.

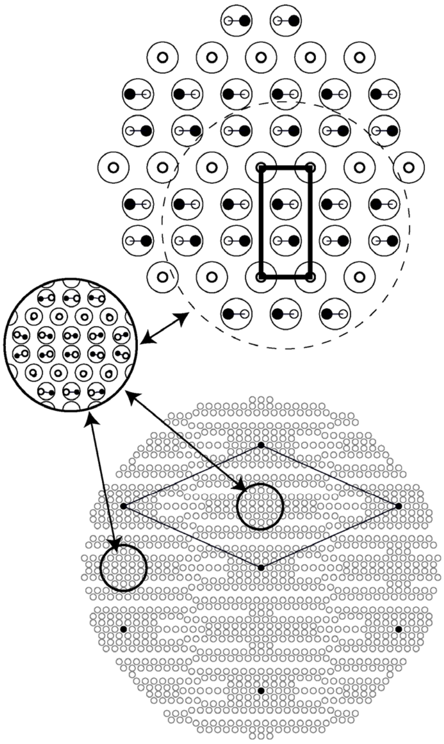

Figure 3. Rotational interfaces of a non cubic lattice defined by the structure matrix of equation 16. Top: singular interface ξ= 5 (Σ = 3). Bottom: non singular interface ξ = 5 + 1/3 (Σ = 301). Small open and filled circles (dichromatic pattern) identify points of the rotated and unrotated lattices. The length of the lines joining dichromatic pattern points reveals the magnitude of the strain field. Large circles are drawn in the middle of dichromatic points whose distance is smaller than one atomic diameter and represent zones of relatively low strain. Note the non-songular interface contains geometrical features belonging to the singular interface. The rectangle on the top and the rhomus at the bottom are the corresponding CSL unit cells.

$$\boldsymbol{L}=\begin{pmatrix}1 & -1/2\\ 0 & \sqrt{5}/2\end{pmatrix} \tag{16}$$

The Figure shows that the singular interface has a much simpler structure and that the non singular case has structural units already presented in the singular one in accordance with previous observations [4].

6. Conclusions

We have shown that the expression $\theta=2\tan^{-1}\left(y\sqrt{N}/x\right)$ derived by Ranganathan to calculate the angles at which there exists a CSL for rotational interfaces in the cubic system can also be applied to general (oblique) two-dimensional lattices provided that the quantities σ^2 and $\sigma/\cos(\alpha)$ are rational numbers, with $\sigma=|\boldsymbol{b}|/|\boldsymbol{a}|$ and α is the angle between the basis vectors $\boldsymbol{a}$ and $\boldsymbol{b}$. Note that in contrast with Ranganathan's results, N given by $N=\tan^2(\alpha)$ needs no longer be an integer. Additionally, we have shown that in order for two dimensional lattices to give rise to a (twist) CSL and the basis vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ must have the form $\boldsymbol{a} = (1,0), \boldsymbol{b} = \left(1, \sqrt{N}\right)$, where r is an arbitrary rational number.

We have also shown that the interfacial classification based on the recurrence properties of the O-lattice remains valid for arbitrary two-dimensional interfaces provided the above requirements on the lattice are met.

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