Frank's Formula

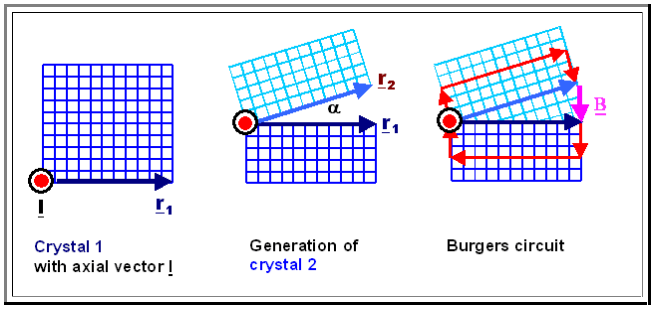
Advanced

Note: For ease of writing /reading in this module, variables are not in *italics*; instead vectors are underlined

- Franks formula relates **B**, the sum of all the specific Burgers vectors $\underline{b}_i$ cut by a vector **r** lying in the plane of the boundary, to the angle α with which one of the crystals is rotated with respect to the other one around the polar unit vector **l**. It is valid for small angles (say $\alpha < 10^o$) and given by

$$\underline{B} = (\underline{r} \times \underline{l}) \cdot \alpha$$

  - Note that we do not need three angles of rotation as required for a general grain boundary because we do not rotate around the axis of a coordinate system, but around the *polar vector* **l**.
  - Note also that the grain boundary plane (and thus **r**) is *not* required to be perpendicular to **l**. **r** thus can have *any* direction and length relative to **l**.
- For the derivation of Franks formula we consider a small angle grain boundary formed by rotating crystal **1** around an arbitrary axis **l** by α and thus forming crystal **2**. After that we join crystal **1** and crystal **2** on *any* plane.
  - A vector $\underline{r}_1$ in the plane of the grain boundary (to be) in crystal **1** thus gets transformed to a vector $\underline{r}_2$ in crystal **2**. Note that $\underline{r}_1$ does not have to be perpendicular to **l**.
  - Next, we make a Burgers circuit in the system with the small angle grain boundary and a reference circuit in the perfect crystal **1** (or crystal **2**). We will move along a vector $\underline{r}_1$ that is much longer than a lattice constant or the spacing of the dislocations that will make up the boundary.
  - In the perfect lattice we will start from the endpoint of $\underline{r}_1$ and move to the start of $\underline{r}_1$ in an e.g. counter-clockwise direction. In the crystal with the grain boundary, we do the same circuit, except that as soon as we switch over to grain **2**, we follow $\underline{r}_2$.
  - The whole procedure can be illustrated as follows:



  - There will be a closing failure **B** which must be identical to the sum of the Burgers vectors of all the dislocations contained in the circuit. Only the *components* of the **b**'s lying in the plane perpendicular to **l** are counted, of course.
  - For clarity, the vectors **r** are at right angles to **l** in the drawing, but this is not generally necessary.
- From vector calculus we know that a rotation can be described by an axial vector given by $\underline{R} = \underline{l} \cdot \alpha$.
  - The difference vector **B** between the two vectors $\underline{r}_1$ and $\underline{r}_2$ (with $\underline{r}_2$ produced from $\underline{r}_1$ by the rotation) than can be written as

$$\underline{B} = \underline{r} \times \underline{R}$$

$$= \alpha \cdot (\underline{r} \times \underline{l})$$

  - - and this is Franks formula from above.
- Note that there are two approximations in this. First, we assume *small angles* so that $\sin(\alpha) \approx \alpha$; and secondly, in the same vein, we assume $\underline{r}_1 \approx \underline{r}_2 = \underline{r}$.
  - Of course, we also assume that there is a smooth cross-over at the boundary (or that **r** is so large that to give or take parts of a lattice constant doesn't matter).
- This is a simple formula, but like most vector formulas, it has some hidden power. Before we look into the power of Franks formula a little more closely, we will consider what it *cannot* do:

- The formula gives the *net* content of Burgers vectors in a small angle grain boundary, but *not necessarily the arrangements of the dislocations*. It does not, of course, say anything about possible splitting into partial dislocations either. This means that there might be several arrangements of dislocations with the same **B**. The one that will be observed will be (most likely) the one with lowest total energy.
- No elastic distortion is considered. Between the dislocation the lattice is perfect; elastic distortion is present only in the core regions of the dislocations.

Bearing this in mind, lets look at some special cases. Since Burgers vectors are translation vectors of the lattice, *in general* three sets of non-coplanar dislocation will be required to produce the vector **B**. *Special cases* therefore are boundaries where only one or two sets of dislocations are needed.

If we have a boundary where *one* set of dislocations with Burgers vector $\underline{\mathbf{b}}_1$ is sufficient, **B** can be written as

$$\underline{\mathbf{B}} = N \cdot \underline{\mathbf{b}} = \alpha \cdot (\underline{\mathbf{r}} \times \underline{\mathbf{l}})$$

- With **N =** number of dislocations cut by **r**

This obviously, looking at Franks formula, requires **b** to be perpendicular to **r** and **l**.

- The direction of **r** in the plane of the boundary is arbitrary; this means that **b** must be at right angles to the plane of the boundary or parallel to the normal **n** of the boundary plane and **l** must be at right angles to **n**; it follows that **l** must be contained in the boundary.
- If we now chose the particularly simple case of $\underline{\mathbf{r}} = \underline{\mathbf{r}}_p$ being parallel to **l**, we obtain $(\underline{\mathbf{r}}_p \times \underline{\mathbf{l}}) = 0$, which means that no dislocations are intersected by $\underline{\mathbf{r}}_p$, implying that the dislocation lines must be parallel to the rotation axis **l**.

This leaves room only for the conclusion that *a boundary with only one set of dislocations must be a pure tilt boundary*.

- The spacing of the dislocations is obtained if we take $\underline{\mathbf{r}} = \underline{\mathbf{r}}_{ra}$ at right angles to **l** thus intersecting the dislocations lines at right angles, too. In this case we can write $\underline{\mathbf{r}}_{ra}$ as $\underline{\mathbf{r}}_{ra} = \mathbf{r} \cdot (\underline{\mathbf{l}} \times \underline{\mathbf{n}})$ and obtain

$$\begin{aligned} N \cdot \underline{\mathbf{b}} &= \alpha \cdot (\underline{\mathbf{r}} \times \underline{\mathbf{l}}) \\ &= \alpha \cdot r \cdot [(\underline{\mathbf{l}} \times \underline{\mathbf{n}}) \times \underline{\mathbf{l}}] \\ &= \alpha \cdot r \cdot \underline{\mathbf{n}} \end{aligned}$$

- With $\underline{\mathbf{b}} = \mathbf{b} \cdot \underline{\mathbf{n}}$ and the spacing **d** between the dislocations given by **d = r/N**, we obtain for the spacing $\mathbf{d}_{tilt}$ of dislocations in a pure tilt boundary with the boundary plane at right angles to the Burgers vector the relation used before:

$$d_{tilt} = \frac{b}{\alpha}$$

Similar considerations, which are straight forward but quite involved, can be made for the case of small angle grain boundaries with *two sets of dislocations* and the possible subsets (e.g. Burgers vectors in the plane of the boundary for pure twist boundaries).

- For this and more, Hull and Bacons book can be consulted, which treats these cases in detail.

More important in the development of boundary structure theories is Bollmanns interpretation of Franks formula; which is the starting point of the **O**-lattice theory as will be discussed in the link.