

Frank's Formula

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

Advanced

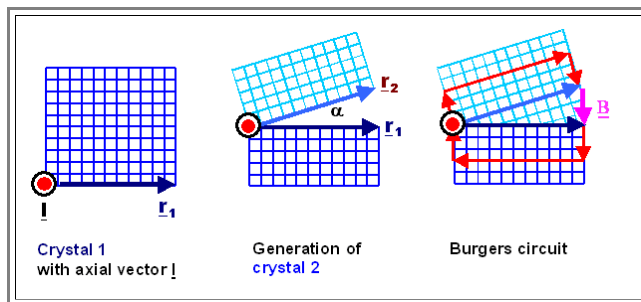
Franks formula relates \underline{B} , the sum of all the specific Burgers vectors \underline{b}_i cut by a vector \underline{r} lying in the plane of the boundary, to the angle α with which one of the crystals is rotated with respect to the other one around the polar unit vector \underline{l} . It is valid for small angles (say $\alpha < 10^\circ$) 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* \underline{l} .
- Note also that the grain boundary plane (and thus \underline{r}) is *not* required to be perpendicular to \underline{l} . \underline{r} thus can have *any* direction and length relative to \underline{l} .

For the derivation of Franks formula we consider a small angle grain boundary formed by rotating crystal 1 around an arbitrary axis \underline{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 \underline{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 \underline{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 \underline{b} 's lying in the plane perpendicular to \underline{l} are counted, of course.
 - For clarity, the vectors \underline{r} are at right angles to \underline{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 \underline{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 \underline{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 $\underline{\mathbf{B}}$. 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, let's 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 $\underline{\mathbf{B}}$. *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, $\underline{\mathbf{B}}$ can be written as

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

- With \mathbf{N} = number of dislocations cut by $\underline{\mathbf{r}}$

▶ This obviously, looking at Franks formula, requires $\underline{\mathbf{b}}$ to be perpendicular to $\underline{\mathbf{r}}$ and $\underline{\mathbf{l}}$.

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

▶ 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 $\underline{\mathbf{l}}$ thus intersecting the dislocations lines at right angles, too. In this case we can write $\underline{\mathbf{r}}_{ra}$ as $\underline{\mathbf{r}}_{ra} = \underline{\mathbf{r}} \cdot (\underline{\mathbf{l}} \times \underline{\mathbf{n}})$ and obtain

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

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

$$\underline{\mathbf{d}}_{\text{tilt}} = \frac{\underline{\mathbf{b}}}{\alpha}$$

▶ 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 Bacon's](#) book can be consulted, which treats these cases in detail.

▶ More important in the development of boundary structure theories is [Bollmann's interpretation](#) of Franks formula; which is the starting point of the [O-lattice theory](#) as will be discussed in the link.