Bollmanns Interpretation of Frank's Formula

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

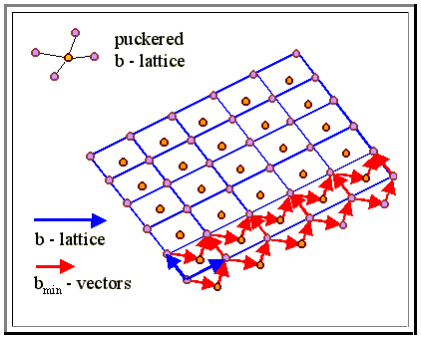
Frank's Formula Reconsidered

Advanced

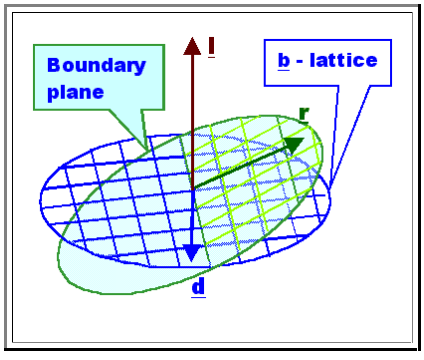
- Franks formula relates the sum **B** of all Burgers vectors cut by a vector **r** (which is required to be in the plane of the boundary) to the (small) rotation angle α around an arbitrary polar vector **l** that generates the second crystal from the first one. It states:

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

- Franks formula at this point is a *continuum equation*, it gives a value of **B** for every α and **r**
  - Burgers vectors, however, are *discrete*. This requires the vector **B** to be discrete, too.
  - Since Burgers vectors are translation vectors of the lattice, **B** can only be a sum of Burgers vectors.
  - If **l** is a lattice vector so that the "**b**-plane", the plane perpendicular to **l** that contains the possible Burgers vectors, is a lattice plane, too (i.e. it can be indexed with **{hkl}**, with **h, k, l** = integers). It contains lattice points that define the possible Burgers vectors in this plane.
  - Note that the Burgers vectors defined in this way must not necessarily be the shortest possible Burgers vectors $\mathbf{b}_{min}$, i.e. the Burgers vectors of real dislocations. It is, however, always possible to decompose the **b** vectors of the **b**-lattice into e.g., **a/2<110>** type Burgers vectors of the **fcc** lattice. This may require $\mathbf{b}_{min}$-vectors that are *not* contained in the **b**- plane - but all we have to do then is to imagine the net of **b**-vectors in this plane to be "puckered" as shown below.



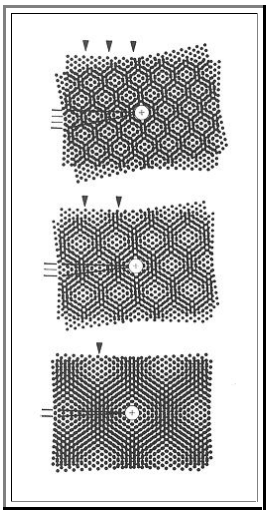
- In the plane of the boundary, an arbitrary **r** would intersect the projection of the **b**-lattice onto the boundary plane along the **l**-direction. In a schematic view we have the following situation:



- Franks formula can now be understood as a *discrete imaging of points in a two-dimensional "Burgers vector space" onto a plane in real space*.
  - The Burgers vector count along **r** (after translating it to smallest possible vectors $\mathbf{b}_{min}$) gives the number of dislocations that are found if going along **r** in the boundary plane. If even spacing is assumed, we also know the spacing in the particular direction given by **r**.
- Now comes something new. Remember that Franks formula did not make any statement about the arrangement of the dislocations, or - in other words - their line direction.
  - Bollmanns view is different: The line direction of the dislocation is obtained by probing the whole two-dimensional grain boundary space by sweeping **r** around. What happens then can be understood in purely geometrical terms, as we will see below.

Bollmanns view of Frank's Formula

First of all it is important to realize that the crossing of a dislocation by the "probing" vector **r** in the **b**-plane is directly imaged by the **Moirée pattern** of the superimposed two crystals obtained by rotating the **{hkl}** planes perpendicular to **l** on top of each other by α as shown below for three different α**s** with pictures from Bollmanns book.



- In the whitish (bright) areas, there is a high degree of coincidence of lattice points, whereas in the black areas the misfit is largest. These are of course the "**O**-points" in the full **O**-lattice theory.
- Whenever a vector from the origin crosses a black area to reach a whitish area again, the translation relative to an equivalent vector in the other lattice is just a lattice vector of the underlying plane, which is the **b**-plane in our definition. In other words, if you move to the same white area in crystal **I** and crystal **II**, the two vectors are on top of each other. But their tips would be separated by just a lattice vector if you now rotate the crystals back to a no-boundary situation.
- If the crystal now introduces a boundary, it will increase the whitish areas, the areas of best fit, and concentrate the misfit in the black areas - which correspond to the dislocations. A periodic structure results which we can describe as a lattice - the (**2**-dimensional) **b-lattice**.
- Since the Moirée pattern does not depend on the position along **l**, we can extend the **b**-lattice along the **l** direction and obtain a **3**-dimensional structure with lattice lines instead of points. If we enclose the lattice points (respectively lines) of the **b**-lattice in **Wigner-Seitz cells**, we obtain a kind of honeycomb structure.

The decisive point now is that the *boundary plane*, which can have *any* position relative to **l**, intersects this "honeycomb" **b**-lattice somehow, for an arbitrary case we obtain the following picture (again taken from Bollmanns book)

- The **b**-lattice consists of the yellow lattice points. It is turned into the three-dimensional "honeycomb" lattice by introducing Wigner-Seitz cells (blue lines) and continuing it along the **l** direction (magenta arrows). The lines would be the **O**-lattice in the full theory.
- An inclined boundary plane will have a dislocation wherever the boundary plane intersects the honeycombs. The resulting dislocation network is shown with red lines. The points of best fit (red points) are in the center of the network as it must be.
- The final network may still be different because the Burgers vectors of the dislocations now defined by the "red lines" might be too large and decompose, as pointed out above.

The final interpretation now is as follows:

- Wherever the boundary plane intersects a cell wall of the (three-dimensional) **b**-lattice, we have a dislocation with the Burgers vector as defined by the translation vectors in the **b**-lattice. The lines defined by the intersection of the boundary plane and the cell walls then directly define the dislocation lines - we get a direct rendering of the dislocation network in the boundary.
- Of course, the geometry of the dislocation network obtained in this way depends on the kind of unit cell we chose for the "honeycomb" **b**-lattice. Wigner-Seitz cells, while universal, may not be best choice possible. But it is always possible now to "develop" the network obtained to a *network with minimum energy* by using the rules of dislocation interaction as in the example with the small angle twist boundary on a **{111}** plane.

These and other complications need more considerations. However, remembering that Franks formula is an approximation and covers only small angle grain boundaries, it is not worth the effort to improve this limited theory. It is a better at this point to unleash the full power of **O**-lattice theory which contains Franks formula as a special case.

The concepts behind Bollmanns interpretation of Franks formula are not easy and lead into very deep water. Let's recapitulate the essential ideas:

- The orientation relationship between the two crystals (expressed here as *one* rotation) always leads to a kind of Moirée pattern that can be identified as a Burgers vector lattice (**b**-lattice) describing the localized displacements necessary to match the two crystals on some boundary plane.
- The **b**-lattice can be extended to three dimensions (the "honeycomb" lattice for the case treated here). The cell walls of this three-dimensional lattice define the dislocation content of the boundary and the Burgers vectors encountered in crossing a wall.
- The intersection lines obtained by cutting the three-dimensional **b**-lattice with the boundary plane defines directly the dislocation network.