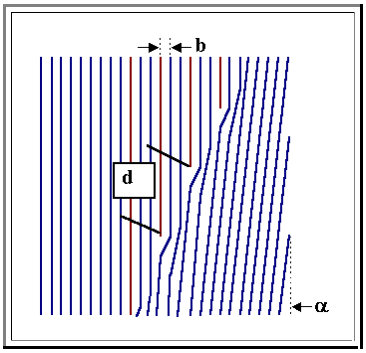
7.2.2 Case Studies: Small Angle Grain Boundaries in Silicon I

First we will take a close look at some small angle grain boundaries in Silicon. Whereas they are the most simple boundaries imaginable, they are still complex enough to merit some attention. They are also suitable to demonstrate a few more essential properties of grain boundary dislocations.

- Lets first look at a pure tilt boundary as outlined in the preceding paragraph. Below is shown how edge dislocations can accommodate the misfit relative to the **Σ = 1** orientation (for a boundary plane that contains the dislocations lines).

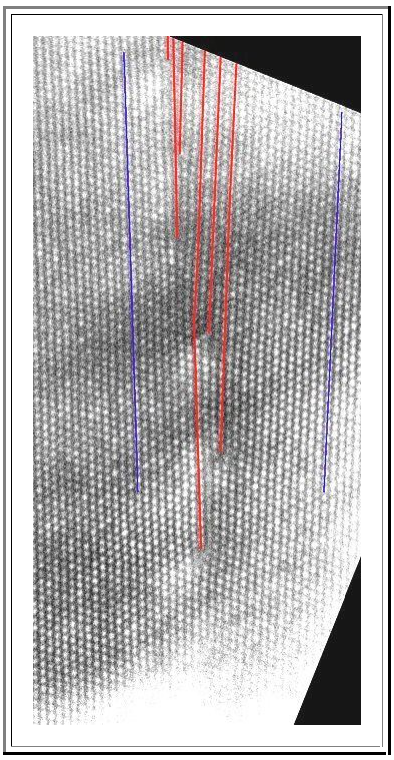


- The distance ***d*** between the dislocations is for small tilt angles α as before given by

$$\alpha = \frac{d}{b}$$

- This is a simple version of a general relation betwen Burgers vectors and misorientation in small angle grain boundaries called **Franks formula** (more correctly Frank-**Bilby** formula).

- In real life it looks slightly more complicated - but not much:

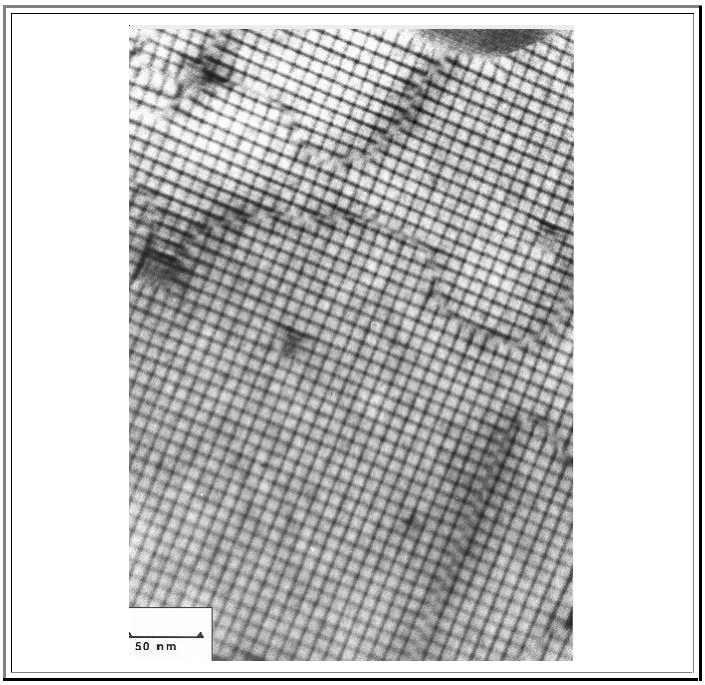


- This is an early **HRTEM** of a small angle tilt boundary in **Si**. The red lines mark the edge dislocations, the blue lines indicate the tilt angle.

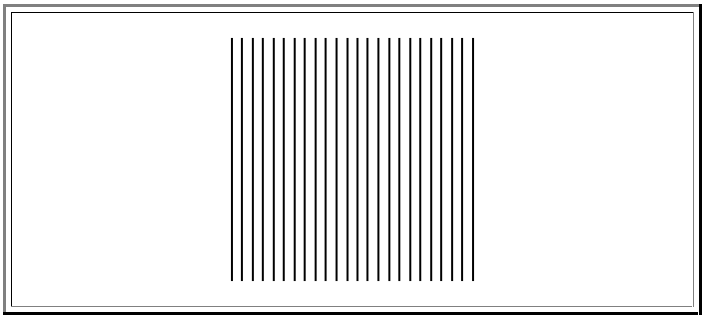
- This picture nicely illustrates that we have indeed a **Σ 1** relationship in the area between the dislocations, i.e. a perfect crystal. The dislocations are not all in a row, but that does not really matter.

Next, we look at twist boundaries.

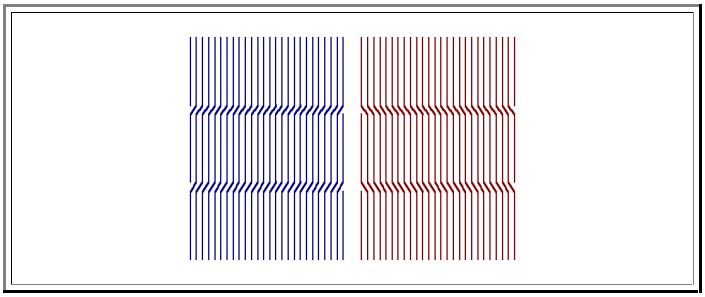
- These and some of the other boundaries were artificially produced to study the structure. Two specimens of **Si** with a desired orientation relationship were placed on top of each other and "sintered" or "welded" together at high temperatures. This process, first called "sintering" is now known as "**waferbonding**" and used for technical applications.
- The result for a slight twist between **{100}** planes is shown in the next picture:



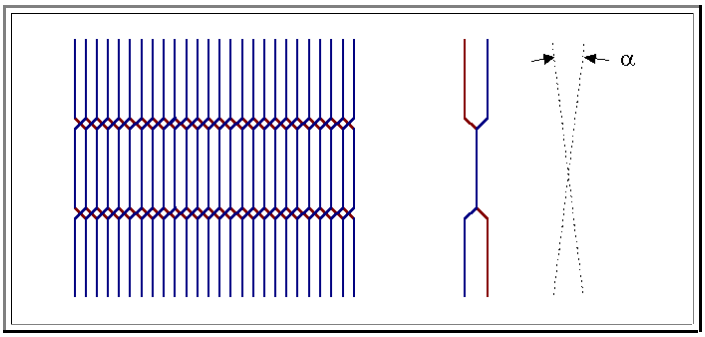
- This is a remarkable picture. As ascertained by contrast analysis, it shows a square network of *pure screw dislocations* . The picture is remarkable not only because it shows a rather perfect square network of screw dislocations, but because it is obviously a **bright field** **TEM** micrograph, however with a resolution akin to **weak-beam** conditions.
  - Pictures like this one are obtained by orienting the specimen close to a **{100}** (or, in other cases, **{111}**) orientation thus exciting many reflections weakly. All dislocations are then imaged, but the detailed contrast mechanism causing the superb resolution is not too clear.
- Lets first find out why a network like this can produce the required twist. We do this in reverse order, i.e. we will construct a screw dislocation network in a perfect crystal and see what it does.
  - We start by looking at **{100}** lattice planes below and above the (future) grain boundary plane. They are exactly on top of each other, we obtain a (trivial) picture of a formal low-angle twist boundary with twist angle α **= 0°**.



  - Now we introduce two screw dislocations running from left to right. Referring to the same kind of picture in chapter 5, we see that the lattice planes below the screw dislocations are bent to the right (blue lines), above the screw dislocations to the left:



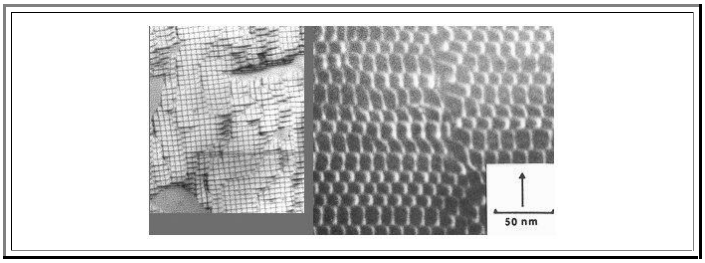
With many dislocations, the average orientation of the lattice planes below the small angle grain boundary will rotate to the right, above to the left. The combined effect is shown below.



- If we want to rotate not just one set of lattice planes, but all of the top part of the crystal, we need at least a second set of screw dislocations. This produces a screw dislocation network of the kind shown in the **TEM** micrograph above.
  - The relation between the twist angle α and the dislocation spacing ***d*** is again a simple version of the general case given in Franks formula:

$$\alpha = \frac{b}{d}$$

  - A detailed drawing of this dislocation network structure can be viewed in the link.
  - With luck, it is possible to image the lattice plane in a **HRTEM** micrograph. The link shows examples - the only **HRTEM** image of screw dislocations obtained so far.
- The exact geometry of the network for the same twist angle α in an *arbitrary* twist boundary depends on many factors:
  - The *twist angle α* which determines the spacing between the dislocations. For **Σ = 1** boundaries it simply the twist angle itself, for arbitrary boundaries it is the twist angle needed to bring the boundary to the closest low **Σ** orientation
  - The *Burgers vectors* of the dislocations. Even in small-angle grain boundaries they could be perfect, or split into partials. In arbitrary boundaries they must be grain boundary dislocations with a Burgers vector of the proper **DSC** lattice. Note that a network of *grain boundary* screw dislocations simply superimposes some twist to whatever orientation the boundary has without those dislocations.
  - The *type of the dislocations*. For an arbitrary twist plane, the Burgers vectors of the possible dislocations are not necessarily contained in the grain boundary plane; the required pure screw dislocations do not exist. In this case mixed dislocations must be used with a component of the Burgers vector in the grain boundary plane.
  - The *symmetries* of the two crystal planes in contact at the grain boundary - even low-angle twist boundaries with a twist around the **<100>** axis can be joined on planes other than **{100}**.
  - The complications that may arise because the (perfect) *dislocations split into partials*. Obviously, that has not happened in the case shown above. The reason most likely is that the splitting would have to be on two different **{111}** planes inclined to the boundary plane (look at your Thompson tetrahedron!) which leads to very unfavorable knot configurations. Since the distance between dislocations is of the same order of magnitude as the typical distance between partials, we do not observe splitting into partials or dissociation of the knots.
- We now can understand the very regular square network shown in the picture above - it is really about the most simple structure imaginable.
  - But we still need to explain the interruptions in the network; the lines along which the net is shifted. In fact, to see a very regular network like this you must be pretty lucky; more often than not often (artificially) made twist grain boundaries look like this:



  - Both pictures show the result of the attempt to make a pure twist boundary. Whereas the left one still looks like the picture above - just with more interruption of the network - the right one does not convey the impression of a square network at all.
  - The answer is that these grain boundaries must accommodate more that just a pure twist: There is also a tilt component and the plane of the grain boundary is not exactly **{100}**. We will pick up this subject again in the next paragraph; more information about the right-hand side picture can be found in the link.