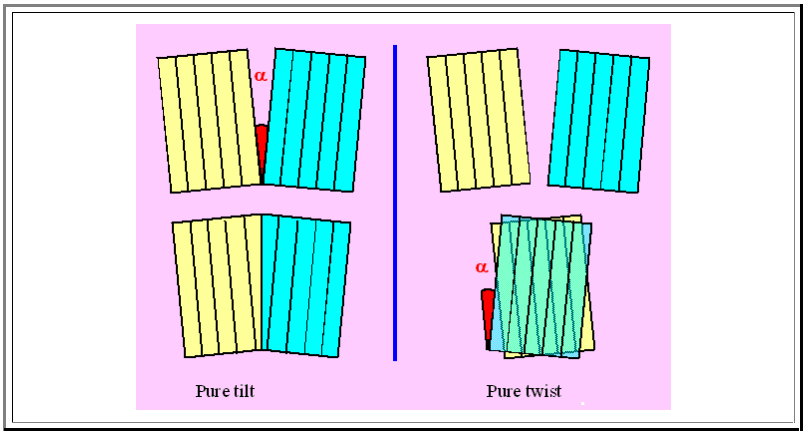
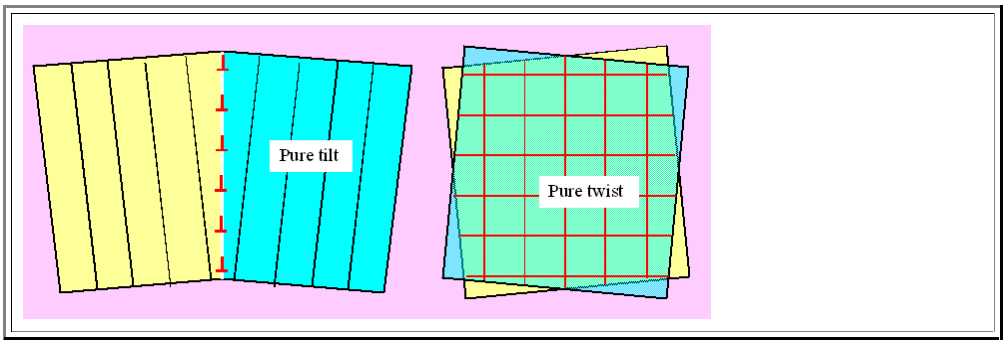
7.2 Grain Boundary Dislocations

7.2.1 Small Angle Grain Boundaries and Beyond

- The determination of the precise dislocation structure needed to transform a *near-coincidence* boundary into a *true* coincidence boundary with some superimposed grain boundary dislocation network can be exceedingly difficult (to you, not to the crystal), especially when the steps possibly associated with the grain boundary dislocations must be accounted for, too.
  - Nevertheless, the structure thus obtained is what you will see in a **TEM** picture - the crystal has no problem whatsoever to "solve" this problem!
- In order to get familiar with the concept, it is easiest, to consider the environment of the **Σ= 1** grain boundary, i.e. the boundary between two crystals with *almost* identical orientation.
  - This kind of boundary is known as "**small-angle grain boundary**" (***SAGB***) , or, as already used above as "**Σ1** boundary".
  - We can easily imagine the two extreme cases: A pure tilt and a pure twist boundary; they are shown below.



  - Obviously, we are somewhat off the **Σ 1** position. Introducing grain boundary dislocations now will establish the exact **Σ1** relation between the dislocations (and something heavily disturbed at the dislocation cores). The **DSC**-lattice as well the **CSL** are identical with the crystal lattice in this case, so the grain-boundary dislocations are simple lattice dislocations.
  - Introducing a sequence of edge dislocations in the tilt case and a network (not necessarily square) of screw dislocations in the twist case will do the necessary transformation; this is schematically shown below



- This may not be directly obvious, but we will be looking at those structures in great detail in the next paragraph. Here we note the important points again:
  - Between the dislocation lines we now have a *perfect **Σ1** relation* (apart from some elastic bending).
  - All of the misfit relative to a perfect Σ orientation is concentrated in the grain boundary dislocations.
  - We thus *lowered* the grain boundary energy in the area between the dislocations and *raised* it along the dislocations - there is the possibility of optimizing the grain boundary energy. The outcome quite generally is:
- Grain boundaries containing grain boundary dislocations which account for small misfits relative to a preferred (low) Σ orientation, are in general preferable to dislocation-free boundaries.
  - The Burgers vectors of the grain boundary dislocations could be translation vectors of one of the crystals, but that is energetically not favorable because the Burgers vectors are large and the energy of a dislocation scales with Gb^2 and there is a much better alternative:
  - The dislocations accounting for small deviations from a low Σ orientation are *dislocations in the **DSC** lattice* belonging to the *CSL lattice* that the grain boundary Σ endeavors to assume. Why should that be so? There are several reasons:

1. Dislocations in the **DSC** lattice belong to *both* crystals since the **DSC** lattice is defined in both crystals.
2. Burgers vectors of the **DSC** lattice are smaller than Burgers vectors of the crystal lattice, the energy of several **DSC** lattice dislocations with a Burgers vector sum equal to that of a crystal lattice dislocations thus is always much smaller. With
   $\Sigma_i \, \boldsymbol{b}_i\mathbf{(DSC)} = \boldsymbol{b}\mathbf{(Lattice)}$, we always have
   $\Sigma_i \, \boldsymbol{b}_i^2\mathbf{(DSC)} << \mathbf{b^2(Lattice)}$.
   This is exactly the same consideration as in the case of lattice dislocations split into partial dislocations.
3. A dislocation arrangement with the same "*Burgers vector count*" along some arbitrary vector ***r*** produces exactly the same displacement (remember the basic Volterra definition and the double cut procedure).

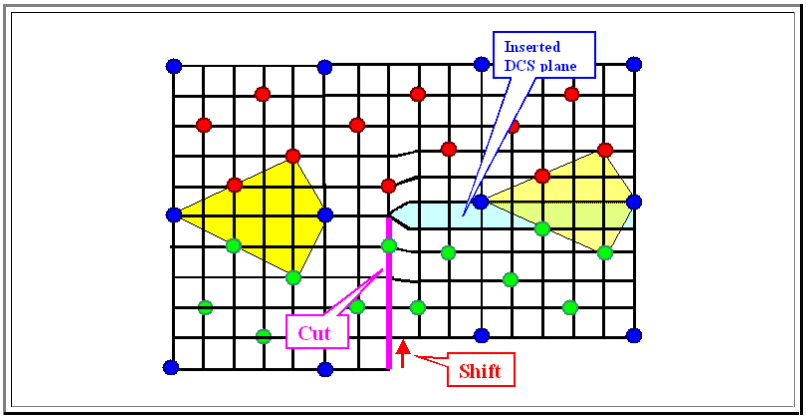
In other words: We can always imagine a low angle boundary of crystal lattice dislocations that produces exactly the small misorientation needed to turn an arbitrary boundary to the nearest low Σ position and superimpose it on this boundary.

Next, we decompose the crystal lattice dislocations into dislocations of the **DSC** lattice belonging to the low Σ orientation.

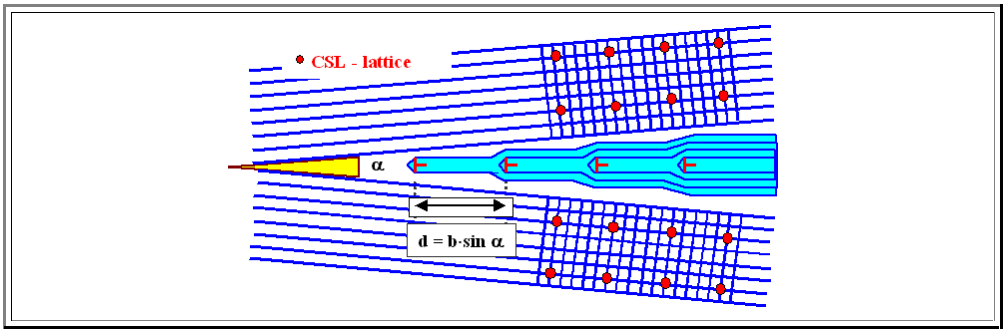
This will be the dislocation network that we are going to find in the real boundary!

Lets illustrate this. First we construct another kind of **DSC** lattice dislocation, very similar, but different to the one we had before. The coincidence points are marked in blue, atoms of the two crystal lattices in green and red.

The plane of the cut now is perpendicular to the boundary and extends, by necessity, all the way to the boundary. We produced a **DSC** edge dislocation with a Burgers vector perpendicular to the boundary plane (and a step of the boundary plane).



If we were to repeat this procedure at regular intervals along the boundary, we obtain the structure schematically outlined below.



In essence, we superimposed a tilt component with a tilt angle α that for small angles is given by is given by

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

with ***d*** = spacing of the **DSC** lattice dislocations and ***b*** = Burgers vector of the **DSC** lattice dislocations.

In short, we can do everything with **DSC** lattice dislocations in a grain boundary that we can do with crystal lattice dislocations. This leads to the crucial question alluded to before:

How do we *calculate* the **DSC**-lattice? As an example for the most general case of grain boundaries in triclinic lattices? Or even worse: For *phase boundaries* between two different lattices (with different lattice constants)?

The answer is: Use the "**Bollmann theory** or " **O-lattice theory**" - it covers (almost) everything.

However, unless you are willing to devote a few months of your time in learning the concept and the math of the **O**-lattice theory, you will encounter problems - it is not an easy concept to grasp.

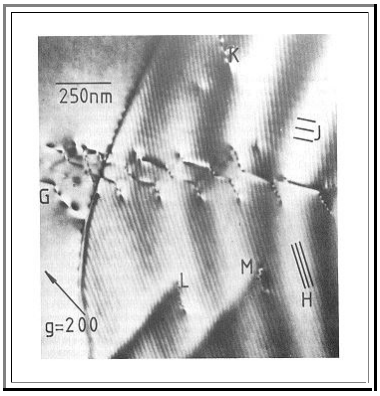
- We will deal with the O-lattice theory in a backbone II section, here we note that the most important cases have been tabulated. Some solutions *for fcc crystals* are given in the table:

Σ	Generation	***b* from DSC-lattice**
1	"Small-angle GB"	a/2 <110>, possibly split into partials
3	Twin	a/6 <112>, a/3 <111>
5	37° around <100>	a/10 <130>
9	39,9° around <110>	1/18<114>, 1/9<122>, 1/18<127>,
19	26,5° around <110>	a/38 <116>, a/19<133>, a/19 <10,9,3>
41	12,7° around <100>	a/82<41,5,4>, a/82<910>, ...

- Interestingly (and very satisfyingly), the **DSC** lattice vectors belonging to the **Σ = 3** boundary are our old acquaintances, the partial Burgers vectors associated with stacking faults in the crystal lattice.
- This is but natural - a **Σ = 3** twin boundary is after all a very close relative to stacking faults.

Now a question might come up: **Σ = 41** is not exactly a "**low Σ**" value; and Burgers vectors of **a/82<41,5,4>** appear to be a bit odd, too. So does this still make sense? Are boundaries close to a **Σ41** orientation still special and bound to have grain boundary dislocations?

- *Only the experiment can tell* . The following **TEM** picture shows a **Σ 41** grain boundary (from Dingley and Pond, Acta Met. **27**, 667, 1979)



- A network of grain boundary dislocations with Burgers vectors **b = a/82 <41,5,4>** and an average distance of **20 nm** is visible. The two sets of dislocations run parallel to the lines indicated by **H** and **J**.
- Sorry, but it is there, even at **Σ = 41**. Why - we do not really know, although Bollmann theory does provide an answer on occasion.

Obviously, if you want to understand the structure of grain boundaries, you must accept the concept of grain boundary dislocations even at rather large values of Σ and correspondingly low values of the Burgers vectors.

In the next paragraph we will study some cases in more detail.