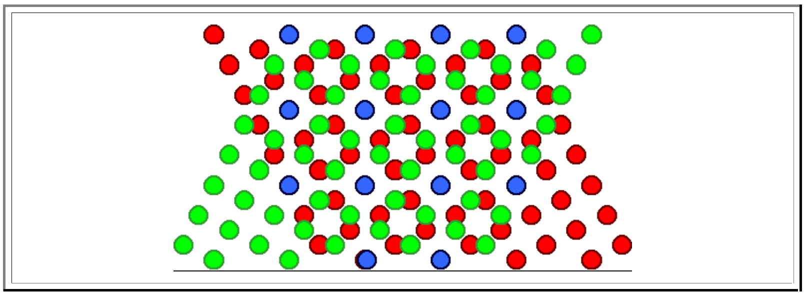
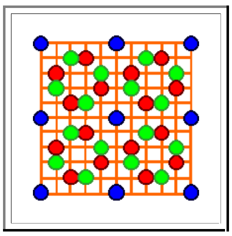
7.1.3 The DSC Lattice and Defects in Grain Boundaries:

- Grain boundaries may contain special defects that *only* exist in grain boundaries; the most prominent ones are **grain boundary dislocations**. Grain boundary dislocations are linear defects with all the characteristics of lattice dislocations, but with very specific Burgers vectors that can *only* occur in grain boundaries.
  - To construct grain boundary dislocations, we can use the universal Volterra definition.We start with a "low Σ" boundary and make a cut in the habit plane of the boundary. The cut line, as before, will define the dislocation line vector ***l*** which by definition will be contained in the boundary.
  - Now we displace one grain with respect to the other grain by the Burgers vector ***b*** so as to preserve the *structure of the boundary* everywhere except around the dislocation line. In other words: the structure of the boundary after the shift looks exactly as before the shift.
- What does that mean? What is the "structure of the boundary" and how do we preserve it?
  - Well, we have a **CSL** on both sides of the boundary. We certainly will preserve the structure of the boundary if we shift by a translation vector of the **CSL**, i.e. by a rather large Burgers vector. We than would preserve the coincidence site *lattice* - which is fine, but far too limited. We already preserve the structure of the boundary if we simply *preserve the coincidence*!
  - It is best to illustrate what this means with a *simple animation*: Two superimposed lattices form a ***CSL** marked in blue*. The red lattice moves to the left, and at first there are no more coincidences of lattice points - the **CSL** has disappeared and we have a different structure. However, after a short distance of shifting - far smaller than a lattice vector of the **CSL**, *coincidence points* appears and we have a **CSL** again - but with the coincidence *points* now in different positions.

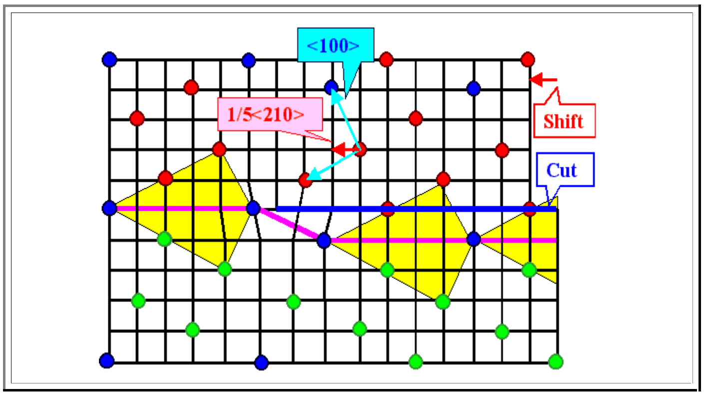


  - We found a displacement vector that preserved the structure of the boundary - sort of experimentally. There are others, too, and the possible displacements vectors that conserve the **CSL** obviously are not limited to vectors of the crystal lattice; *they can be much smaller*. This we can generalize:
- The set of all possible displacement vectors which preserve the **CSL** defines a *new kind of lattice*, the so-called ***DSC*-lattice**. The abbreviation "**DSC**" stands for "*Displacement Shift Complete*", not the best of possible names, but time-honored by now.
  - A better way of thinking about it would be to interprete the abbreviation as "*Displacements which are Symmetry Conserving*". Displacing one grain of a grain boundary with a **CSL** by a vector of the corresponding DSC lattice thus preserves the structure of the boundary because it preserves the symmetries of the **CSL**. We now conclude:
  - *Translation vectors of the **DSC** lattice are possible Burgers vectors* $\mathbf{b_{GB}}$ *for grain boundary dislocations*. As for lattice dislocations, only the smallest possible values will be encountered for energetic reasons.
  - Grain boundary dislocations constructed in this way *by (Volterra) definition*, have most of the properties of real dislocations - just with the added restriction that they are confined to the boundary. Strain- and stress field, line energy, interactions, forming of networks - everything follows the same equations and rules that we found for lattice dislocations.
  - It remains to be seen how the **DSC**-lattice can be constructed. From the illustration it is clear that every vector that moves a lattice site of grain **1** to a lattice site of grain **2** is a **DSC**-lattice vector. This leads to a simple "*working*" definition:
- The **DSC**-lattice is the *coarsest sub-lattice* of the **CSL** that has *all* atoms of *both lattices* on its lattice points. Most lattice points of the **DSC**-lattice, however, will be empty



  - This is the **DSC**-lattice for the animation above. Its easy enough to obtain, *but*:
  - A formal and general definition of the **DSC** lattice (including near **CSL** orientations) is one of the most difficult undertakings in grain boundary theory. If you love tough nuts, turn to chapter 7.3 and proceed.

- Any translation of one of the two crystals along a vector of the orange DSC-lattice will keep the **CSL**, but will generally shift its origin. Only if a **DSC** vector is chosen that is also a vector of the **CSL**, will the origin of the **CSL** remain in place.
- Looking back at the **Σ5** boundary from before, we now can enact the cut and the displacement procedure and generate a picture of the dislocations that must result. The result contains a little surprise and is shown in cross-section below:



- The cut was made from the right. The top crystal (red lattice points) was shifted by a unit vector of the **DSC** lattice, which is a **1/5<210>** vector in both crystal lattices in this case. The second crystal (green lattice points) was left completely unchanged. The coincidence points are blue. We observe two somewhat surprising effects:
- The boundary plane (as indicate by the pink line) after the shift is not identical with the plane of the cut
- The **CSL** has an interruption in both grains - it doesn't fit anymore. Disturbing - *but totally unimportant*. The **CSL**, after all, is *totally meaningless* for real crystals - the (mathematical) coincidence points *in the grains* have no significance for the grains. The *only* significance of a coincidence orientation is that it provides an especially good fit of the two grains at a boundary, i.e. it allows for a particularly favorable boundary *structure*. And the *structure* of the grain boundary is unchanged by the introduction of the grain boundary dislocation, except around its core region. This is indicated by the characteristic diamond shapes (yellow) in the picture above that can be taken as the hallmark of this **Σ5** structure.
- Think about it! Finding the yellow diamonds is the practical way of finding the position of the boundary. However you define the position - you will find the preserved structure as expressed in the yellow diamonds here.
- Introducing the grain boundary dislocation thus had the unexpected additional effect of introducing a **step** in the grain boundary. Some atoms *had to be changed* from green to red to obtain the structure, but that again is an *artifact of the representation*. Real atoms are all the same; they do not come in green and red and do not care to which crystal they belong.

We see that the recipe works: Dislocations in the **DSC** lattice preserve the structure of the boundary; they leave the coincidence relation unchanged. *However*, they also *may* introduce steps in the plane of the boundary -we cannot yet be sure that this always the case.

- Note that is not directly obvious how the step relates to the dislocation, i.e. how the vector describing the step can be deduced from the **DSC** lattice vector used as Burgers vector. (If you see an obvious relationship - please tell me. I'm not aware of a simple formula applicable in all cases).
- Note also: While many (if not all) grain boundary dislocations are linked with a step, the reverse is not true: There are many possible steps in a boundary that do not have *any* dislocation character. More to that in chapter 8.3

The extension to *three dimensions* is obvious, but also a bit mind-boggling. Still, some general rules can be given

- The larger the elementary cell of the **CSL**, the smaller the elementary cell of the **DSC**-lattice!
- If you suspected it by now: The **DSC** lattice is the reciprocal lattice (in space) of the **CSL**.
- The volumes of **CSL**, crystal lattice and **DSC** lattice relate as $\Sigma : 1 : \Sigma^{-1}$ for cubic crystals.

What are all these lattices good for? The main import is:

- A grain boundary between two grains that is *close to, but not exactly at* a low-energy (=low Σ) orientation may decrease its energy if grain boundary dislocations with a Burgers vector of the **DSC** lattice belonging to the low-Σ orientation are introduced so that the dislocation free parts are now in the *precise **CSL** orientation* and all the misalignment is taken up by the grain boundary dislocations.
- We will see how this works in the next sub-chapter.