7.3.5 Pattern Shift and DSC Lattice

The General Idea of Pattern Element Conservation

- In the **CSL** model of grain boundaries the **DSC** lattice was introduced to account for small deviations from a perfect lattice coincidence orientation. It was the lattice of *all translations of one of the crystals that conserved the given **CSL***. Translations other then those of the **DSC** lattice would destroy the coincidence of lattice points.
  - The lattice vectors of the **DSC** lattice therefore could also be interpreted as the set of possible Burgers vectors for dislocations allowed in a grain boundary without destroying the coincidence.
  - While the simple recipe for constructing the **DSC** lattice in the simple cases usually shown (two-dimensional, cubic lattices) is rather straight forward, it was neither mathematically justified, nor is it immediately clear how it should be constructed in complicated cases.
  - The **DSC** lattice, in fact, comes from the **O**-lattice theory and was simply adopted to the "easy" **CSL** model.
- Obviously we now must ask ourselves: What happens to an ***O**-lattice*, particularly a periodic one, if we translate one of the crystals?
  - This is actually one of the more complicated questions to ask, especially for the rank of the transformation matrix **A** **< 3** (as we expect for grain boundaries).
  - We will not go into details here because in this rendering of **O**-lattice theory we omitted some more mathematical points considering what happens to the **O**-lattice in a given situation if you shift (= translate) crystal **I** or crystal **II**. Or, in a reversed situation, how you must shift crystal **I** or **II** if you translate the given **O**-lattice.
- The first answer to the question above is:
  - In general (i.e. rank **A** **= 3**), the **O**-lattice is preserved, but shifted by some amount that depends on the (arbitrary) magnitude of the translation of the crystal chosen. *This is in contrast to the **CSL***, where arbitrary shifts *not* contained in the **DSC** lattice will completely destroy the **CSL**.
  - This does not help, we obviously must find a more specific criterion than just conservation of the **O**-lattice in general in order to find specific translations that correspond to Burgers vectors of grain boundary dislocations. We therefore ask more specifically:
- What happens to the *pattern elements* associated with every equivalence point in a reduced *periodic **O**-lattice* upon shifting one of the crystals?
  - Since we have seen (without proving it) that any **O**-point can be taken as the origin for the rotation transforming crystal **I** into crystal **II**; we should be able to shift lattice **I** by any vector pointing to an equivalence point in the reduced **O**-lattice without changing pattern elements. In other words we simply change the origin of the rotation (we only look at rotations in this examples).
  - The **O**-lattice then will also be shifted by some other vector which can be calculated by employing our basic equation

$$\boxed{(\mathbf{I} - \mathbf{A}^{-1})\, \underline{\mathbf{r}}_{i0} = \underline{\mathbf{T}}(\mathbf{I})}$$

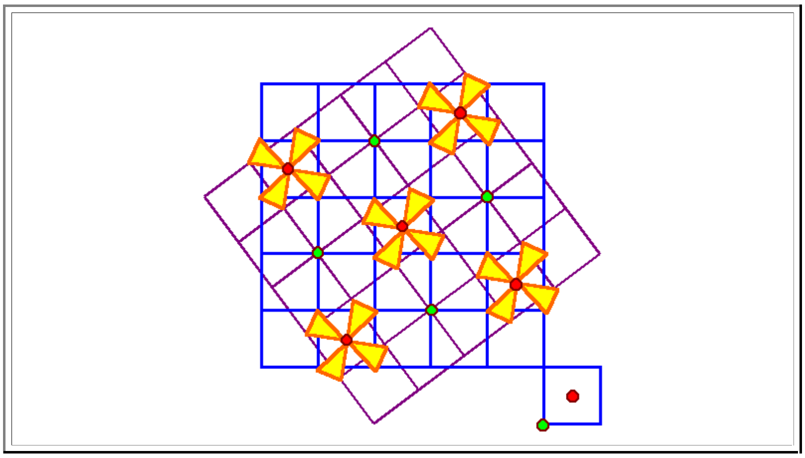
  - The $\underline{\mathbf{r}}_i$ are the base vectors of the **O**-lattice if we take $\underline{\mathbf{T}}_i$ to be the set of base vectors of the crystal **I** lattice.
- Now shift the crystal **I** lattice by some vector $\underline{\mathbf{e}}$ connecting equivalence points, replace $\underline{\mathbf{r}}_i$ by $\underline{\mathbf{r}}_i = \underline{\mathbf{r}}^0_i + \Delta\underline{\mathbf{r}}_i$, with $\Delta\underline{\mathbf{r}}_i$ = shift of the **O**-lattice for a shift $\underline{\mathbf{e}}$ of the crystal lattice, and solve the equation for the $\Delta\underline{\mathbf{r}}_i$.
  - Well, lets *not* do it, but accept that there is a shift that can be calculated.
  - On *second* thoughts, this must also be true for lattice **II**. We thus may also employ vectors that translate lattice **II** by one of the vectors pointing to equivalence points in the reduced **O**-lattice.
  - And on *third* thoughts (not entirely obvious), we also must be able to translate the **O**-lattice itself by any vector that connects equivalence points. This requires that the **O**-lattice shifts by some vector - it is the reverse problem from the one outlined above.
- The trick is that all those shifts may be different, and while they all produce the same general **O**-lattice, there might be different pattern elements. But - there is a *finite* number of pattern elements and a *finite* number of possible shifts.
  - Obviously, the set of all different configurations (distinguished by pattern elements) obtainable defines the complete geometry of the particular boundary with the periodic **O**-lattice considered because no configuration is special.
  - The set of all possible displacement vectors can be expressed as the translation vectors in a new kind of lattice, the "**Complete Pattern Shift Lattice**", abbreviated by Bollmann as " **DSC lattice**", that we encountered earlier (in a much simpler form).
- Unfortunately, it is not immediately obvious how to calculate the **DSC** lattice from **O**-lattice theory. In fact, the respective chapter in Bollmanns book is particularly ***hermetic*** or obtuse.

Somewhat later (**1979**), Bollmann together with **Pond** gave the old abbreviation a new meaning: "**DSC**" now stands for "*Displacements* which are *Symmetry Conserving*". But few people know what exactly **DSC** stands for - the main thing is to understand the significance of the **DSC** lattice.

Some Illustrations

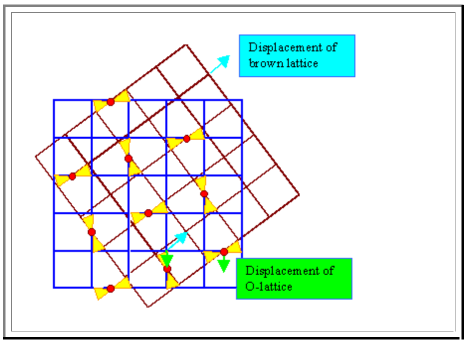
Lets see what the various displacements discussed above really produce if applied to a simple situation. We take the (redrawn) example from Bollmanns book.

- First, lets construct the possible set of pattern conserving translations by putting several reduced **O**-lattice cells together (for the case of rotation around **<100>** of **39^o 52,2'**, corresponding to the **Σ = 5 CSL**).

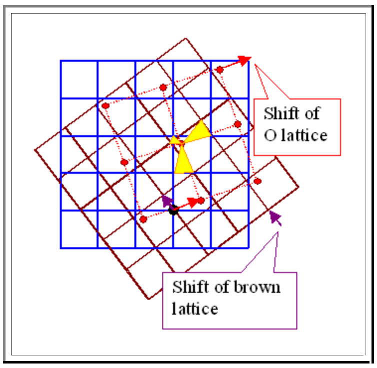


- The left part shows the rotation, yielding the **O**-lattice. Coinciding *lattice* points that are also **O**-points are shown in green, the other **O**-points in red. On the right-hand side the repeated reduced **O**-lattice is shown in the blue crystal.

Now lets displace the brown lattice by a vector pointing form the green to the red equivalence point in the above picture. Here is what you get.



- The **O**-lattice shifted down, and some new kinds of pattern elements appear. There are no more or less special than the ones in the picture above; both belong to the complete structure of the boundary illustrated.
- Note that we also obtain new equivalence points for the boundary (in the middle of the lines defining the square lattices).
- Now we shift the brown lattice by one of the vectors pointing to the new equivalence point. We obtain yet another pattern element.



- But that's it. The pattern elements shown here are all there are (Try to prove that yourself if you don't believe it).
- We could now start to produce the **DSC** lattice, but this will just give the same kind of lattice we had in the simple **CSL** case.

Instead we only note that there is a sufficiently clear procedure of how to create a **DSC** lattice for a given periodic **O**-lattice, that is *always* applicable - even to phase boundaries (in principle; of course only in principle).

- In the next (and last) chapter, we will show how **O**-lattice theory now can be applied to large angle grain boundaries and discuss briefly its merits and limits.