

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 than 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](#)

$$\mathbf{(I - A^{-1}) r_{i0} = T(I)}$$

- The r_i are the base vectors of the **O**-lattice if we take T_i to be the set of base vectors of the crystal **I** lattice.
- ▶ Now shift the crystal **I** lattice by some vector e connecting equivalence points, replace r_i by $r_i = r_i^0 + \Delta r_i$, with $\Delta r_i =$ shift of the **O**-lattice for a shift e of the crystal lattice, and solve the equation for the Δr_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.

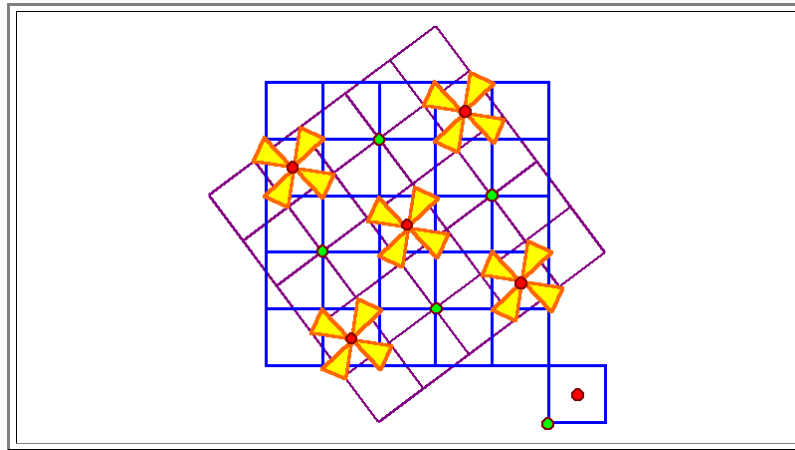
 - Obviously, the set of all different configurations (distinguished by pattern elements) obtainable defines the complete geometry of the particular boundary with the periodic **O**-lattice considered because no configuration is special.
 - The set of all possible displacement vectors can be expressed 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

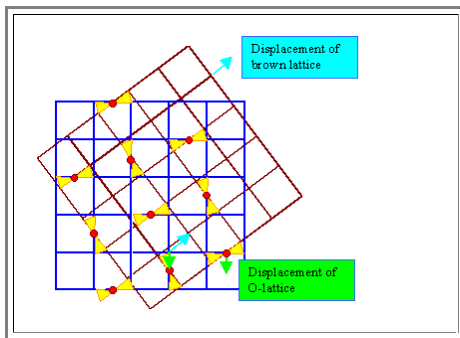
Let's see what the various displacements discussed above really produce if applied to a simple situation. We take the (redrawn) example from Bollmann's book.

- First, let's construct the possible set of pattern conserving translations by putting several reduced O-lattice cells together (for the case of rotation around $\langle 100 \rangle$ of $39^\circ 52,2'$, corresponding to the $\Sigma = 5$ 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.

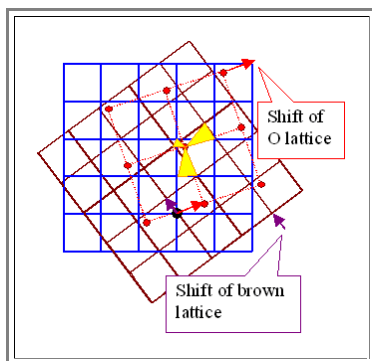
Now let's displace the brown lattice by a vector pointing from the green to the red equivalence point in the above picture. Here is what you get.



- 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.