7.3.6 Large Angle Grain Boundaries and Final Points

Application of O-Lattice Theory to Large Angle Grain Boundaries

- The basic assumption is that an arbitrary grain boundary would prefer to be in a orientation corresponding to a *periodic* **O**-lattice with a high density of equivalence points. This is a fancy (i.e. more general) way for saying that boundaries prefer to be in a low Σ orientation as we did in the simple **CSL** model.
  - Such a particular orientation can be achieved at the expense of generating some *grain boundary dislocations*.
  - For a small angle grain boundary we have seen that a cut of the boundary plane through the **O**-lattice gives directly the geometry of the dislocation network (give or take some adjustments to account for the particular dislocation properties).
  - The **O**-lattice was obtained (by calculations) relative to the two real crystals. Looking back, what we did was to use one of the crystals as a *reference for the preferred state*, the other one then described the *deviation* of the boundary from the preferred state.
- For large angle grain boundaries we now do exactly the same thing - *except* that the reference state is now the *periodic **O**-lattice that the boundary aspires to obtain*.
  - The *deviation* of the boundary from this preferred state is then described by the **O**-lattice that comes with the orientation that describes the *actual* boundary .
- The logical consequence then is that the geometry of the dislocation network necessary to obtain the preferred state is the *__O__-lattice of the two __O__-lattices* described above - a so-called **O2-lattice** or **second order O-lattice**.
  - That may sound a bit heavy, but it is really straight forward if you think about it.
  - It is also clear - in principle - how we would calculate the **O2**-lattice, but we are not going to look at this.
- If we now imagine a boundary plane cutting through our **O2**-lattice as before, we now must ask how large the translation will be that the **O**-lattice "crystals" experience when a **O2**-lattice wall is crossed. This translation will be the Burgers vector of the second-order dislocation forming the grain boundary dislocation network.
  - Well, as you would have guessed, it must be a translation that conserves the underlying pattern of the **O**-lattices, so the translation vector (= Burgers vector) is a vector from the **DSC**-lattice of one of the primary **O**-lattices.
  - While our periodic reference **O**-lattice has a defined **DSC** lattice, the other one may (and in full generality probably will) have a non-periodic **O**-lattice and thus does not have a **DSC** lattice. *This looks like a problem*.
  - However, since **O**-lattices are continuous (and smooth) functions of the misorientation angle (which the **CSL** is not), we know that the two **O**-lattices are rather similar, and we always can take the **DSC** lattice of the periodic **O**-lattice in a good approximation. So there is no real problem.
- OK. We are done. That's (almost) all there is to it.
  - The general recipe for *constructing* a grain boundary with a secondary is network is "clear". It goes exactly along the lines we derived for small angle grain boundaires - only we work in "second order **O**-lattice theory".
  - The reverse is also possible: We have a general recipe for *analyzing* the structure found in a real boundary.
  - It will just take a few months of studying the intricacies of the underlying math and some getting used to the more trickier thoughts, and you can construct and analyze all kinds of boundaries on your own.
- But most likely, you won't. This is due to some (sad) facts of life that will be the last thing to discuss in this context.

Merits and Limitations of O-Lattice Theory

- The merits of Bollmanns theory are clear:
  - It nucleated a lot of work on grain boundary structures and introduced the crucial concept of the **DSC** lattice and its dislocations.
  - It was (and is) the mathematical frame work for tackling the kind of higher-level geometry that is contained in interfaces between crystals. (It will be interesting to see if someone sometime tackles the grain boundary structure between single quasi-crystals, which could be done by extending **O**-lattice theory into a **6**-dimensional space and then project the results back into three dimensional space).
  - It allows to conceive and analyze more complex problems, where a **CSL** model is not sufficient.
- However, there are serious problems and limitations, too.
  - The recipe for the proper choice of the *one* transformation matrix you should use out of many possible ones *is not always correct*. It generally fails for (some) small angle tilt boundaries, where the **O**-lattice theory would predict a twin-like structure with no dislocations - contrary to the observations. It also fails for some other boundaries, casting some lingering doubt on the whole thing.

- It is still *too simple* to account for real boundary structures even if the limitation referred to above does not apply. Two examples might be mentioned.
- **1.** The *rigid body translations* observed in many (twin-like) boundaries, especially in **bcc** lattices.
- **2**. Tremendously complicated structures observed in crystal with more than one atom in the base of the crystal - e.g. in **Si**. What happens (and was first observed and then analyzed by Bollmann) is that dislocations in the **DSC** lattice may split into partial dislocations bounding a stacking fault in the **DSC** lattice. While this effect may be incorporated into the **O**-lattice theory, it does not make it easier.

Still, whereas newer theories concerned with the structures of grain boundaries do exist, none is quite as complete and mathematical as the **O**-lattice theory. A "final" theory has not yet been proposed

What remains for practical work is

- *The **DSC** lattice*. This is certainly the most important outgrowth of the **O**-lattice theory. Grain boundaries simply cannot be discussed without reference to the **DSC** lattice. For practical importance it has all but eclipsed the **O**-lattice. As we have seen, it is (mostly) easily constructed without going into heavy matrix algebra.
- The systematic approach, always good for looking deeper into less clear situations.
- The good feeling, that something can be done about taking a deep look into grain boundary structures from a theoretical point of view, even if there are some limitations and unclear points.