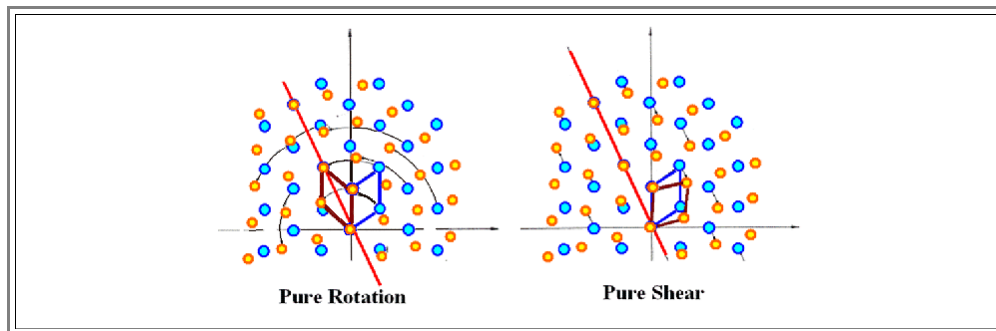## 7.3.2 Working with the O-Lattice

The math and physics of the **O**-lattice is not particularly easy because there are some tricky details to keep in mind. In this paragraph some of the problems, tricks and helpful definitions are just summarized; in due time they may be specified in more details.

It is useful in many cases to decompose the transformation matrix **A** into matrices that describe the *volume deformation* (elongating or shortening only the axes of the crystal), the *shear deformation* (only changing the angles between the axes), and the *rotation* of the coordinate system of crystal **I** separately.

- This may allow a better grasp of the real situation and helps, if necessary, to use approximations only for suitable parts of the system.
- The main reason, however, lies in the fact that the *pure rotation is not unambiguously defined*. Depending on the basic symmetries of the system, the same final state of orientation can be obtained by many different rotations - but only one (or one set) may make sense physically. This leads to the next point:

The choice between various possible transformations **A**. There are many possible ambiguities, not only with respect to the rotation part, but also, e.g., in the relations between pure shear and pure rotation; an example is shown below.

- Starting from a given lattice **I**, identical lattices **II** can be produced either by pure shear or by pure rotation:



Pure Rotation          Pure Shear

*Mathematically*, there is no difference, but *physically* the two transformations are not the same because the atoms involved have to move in quite different ways. Which one is the physically sound one? As it turns out, the criterion is to *preserve nearest neighbor relationships*.

- Mathematically, this means that from all possible transformation matrices **T**, the particular one that has to be chosen is the one *with the smallest numerical value of its determinant |T|*.
- This ensures that the unit cell of the **O**-lattice generated will have the *largest possible value* (it is directly given by **1/|T|**), which will give the smallest possible dislocation content. This requires, of course, that you *know* all the possibilities for **A** in the first place - not a satisfying condition for a mathematician.
- It may be noted in passing, that this *ambiguity* limits the usefulness of the **O**-lattice theory. There are cases, where the choice of the transformation matrix following the rules of **O**-lattice theory, does *not* lead to the "correct" solution as ascertained by looking at what the crystal does (by **TEM**).

Another generalization comes from looking at the essentials of solutions to matrix equations. Consider the solutions of the basic equation

$$(I - A^{-1})\, \underline{r_0} \ = \ \underline{T}$$

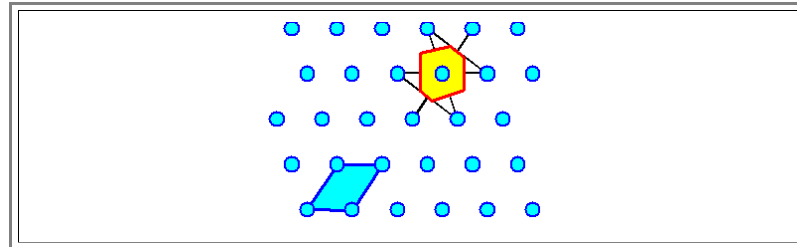- From basic matrix algebra we know that the *type of solution* depends on the **rank** of the matrix **A**.
- We have the following cases:

  - *Rank* **(A) = 3**
    The solutions define *points* in **O**-space, i.e. an **O-lattice**.
  - *Rank* **(A) = 2**
    the solutions are **O-lines**.
  - *Rank* **(A) = 1**
    The solutions are **O-planes**.
  - *Rank* **(A) = 0**,
    we have the trivial case of *identity* **1**.

*This is an issue of prime importance!*.

- Since we can produce *all* grain boundaries (but *not* all phase boundaries) by just rotating crystal **II** around *one* properly chosen axis, the rank of the transformation matrix does not have to be larger than **2**.

- What does this mean? Well - for grain boundaries, there is no such thing as a **O**-point *lattice* - it is rather a *lattice of lines*. We have essentially a *two-dimensional* problem.

- Nevertheless, for the sake of generality, we will continue to discuss the "**O**-point lattice", knowing that it often is just a line lattice.

Solving the basic equation produces the **O**-lattice and therefore also the unit cell of the **O**-lattice. However, the "natural" unit cell obtained by simply connecting **O**-lattice points in some "obvious" manner may not be the physically most sensible one!

- As taught in basic crystallography, there are many ways of defining unit cells - we have another ambiguity!

- We will tend to take the **Wigner**-**Seitz** **cell**. Why? Who knows at this point - just go along. What this means is illustrated below:



- Again, the right choice must come from the physical meaning of the **O**-lattice. This we will discuss in the next paragraph. Here we note that **O**-lattice defined in this way resembles nothing so much as a *honeycomb* - just remember again, that the **O**-points are lines. An illustration that comes fairly close in a slightly different context ("Bollmanns view of Franks formula") can be accessed via the link.