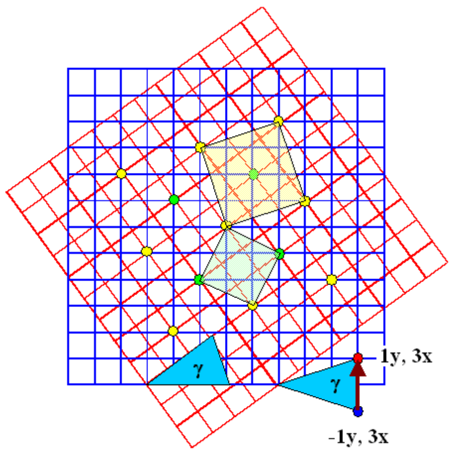
Σ is Always Odd

Advanced

- They most conspicuous issue in the **CSL** theory of grain boundaries is that there are no *even* values for Σ!
  - Try as you might - you will never find a **Σ = 2** boundary or any other *even* number in the literature. Now why is this? Mostly no explanation is given.
- A rigorous proof essentially needs the full power of the **O-**lattice theory, so it can not be easily given. But the general reason for this peculiar geometric fact can be envisioned as follows.
  - First, remember that *any* grain boundary can be obtained by generating grain **II** out of grain **I** by *one* rotation around a suitable axis with the rotation angle γ.
  - This means that we can produce all **CSL** orientations by looking at *one* rotation. We will do this for a square lattice, rotating around a **<100>** axis.
  - It is, however, not obvious that we can indeed produce all possible boundaries by this rotation, nor is it clear that the result will be valid for grain boundaries in non-cubic crystals. But it shows the direction of the argument.
- From all possible rotation, some will produce **CSL** structures. Which ones will do that is easily conceived:
  - The picture below shows a blue crystal **I**. Taking its origin at the apex of the blue triangle on the right, we see that we always will get a **CSL** orientation if we look at lattice points with the coordinates $(x, -y_0)$ which we may express as **(*n*, –1)** if we set $x_0, y_0 = 1$, and than rotate the crystal so the the ***y***-coordinate changes from **–1** to **+1**. The shift is indicated by the bold brown vector; we need to rotate an angle γ given by

$$\gamma = \tfrac{1}{2}\,\text{cotg}\,\frac{y}{x} = 2\cdot\text{cotg}\,\frac{1}{n}$$

  - The red lattice has been rotated by just the right amount to move the point **(3, –1)** to the position **(3, +1)**; the rotation center is in the middle of the crystals



- With this procedure we created the yellow **CSL** lattice.
  - Its **Σ'** value is given by its area divided by the are of a unit cell of the lattice; we have

$$\Sigma' = \frac{(x^2 + y^2)^2}{x_0 \cdot x_0} = \frac{(3x_0)^2 + (1x_0)^2)}{x_0^2} = (3^2 + 1^2) = 10$$

  - Its easy to generalize for **CSL** sites generated by moving the point **(*nx*, –*y*)** on the **(*nx*,+*y*)** position, we obtain for the **Σ'** values

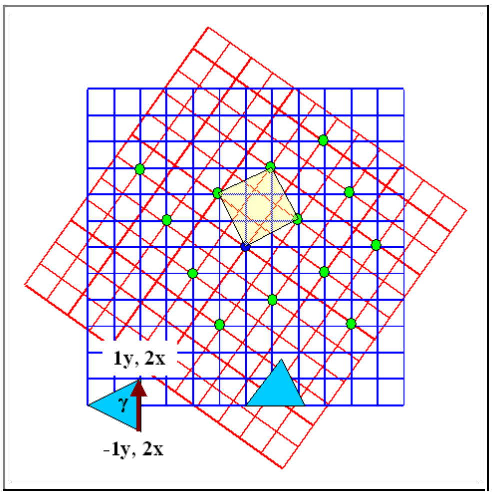
$$\Sigma'(n) = n^2 + 1^2$$

- The result will be
  - **Σ'** is an *odd* number, if ***n*** is an even number (The square of an even number is even plus **1 = odd**)
  - **Σ'** is an *even* number, if ***n*** is an odd number (The square of an odd number is odd plus **1 = even**.)

- So we can get even and odd numbers for Σ????.
  - Yes - but upon inspection you will find that for ***n* = odd**, there is *always* an additional coincidence point in the center of the lattice defined by the **CSL** points produced by the rotation, while for even numbers of ***n*** this is not the case.
  - In the picture above this are the green points, and the lattice constant of the **CSL** lattice is now smaller. The Σ value in this case is simply

$$\Sigma = \frac{n^2 + 1^2}{2^{1/2} \cdot 2^{1/2}} = \Sigma'/2 = \text{an odd number}$$

  - Instead of a **Σ = 10** boundary, we generated a **Σ = 5** boundary and there are no even Σ values.
  - *q.e.d. (sort of)*
- This, of course, is a far cry from a real mathematical proof, but it imparts the flavor of the thinking behind it.
  - To complete this issue, the following picture shows the result for a rotation that tranfers **(2, –1)** to **(2, +1)**



  - There is no additional coincidenc point and we end up with a **Σ = (*n*^{2} + 1^2) = 5** boundary, the same one as above