

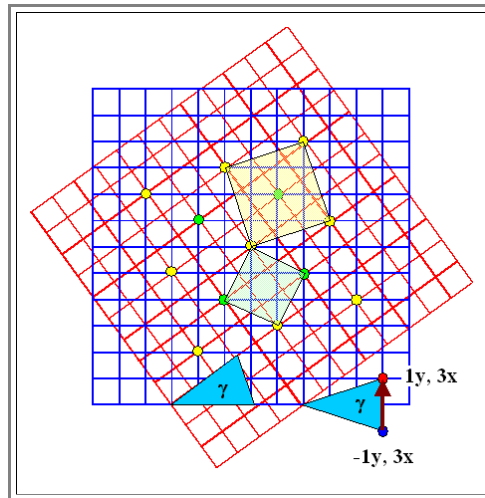
Σ is Always Odd

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, -y₀) which we may express as (n, -1) if we set x₀, y₀ = 1, and then 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

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

- 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 $n = \text{odd}$, 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

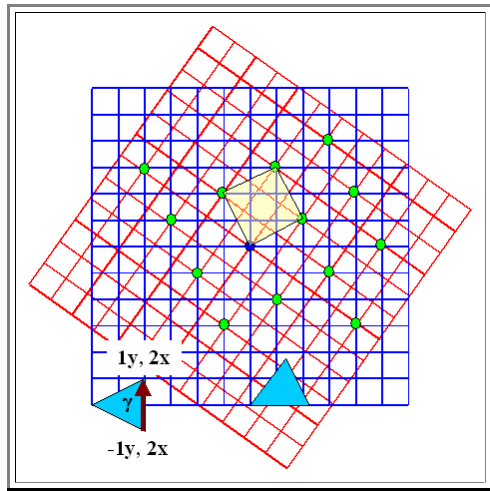
$$\Sigma = \frac{n^2 + 1^2}{2^{1/2} \cdot 2^{1/2}} = \Sigma/2 = \text{an odd number}$$

- Instead of a $\Sigma = 10$ boundary, we generated a $\Sigma = 5$ 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 transfers $(2, -1)$ to $(2, +1)$



- There is no additional coincident point and we end up with a $\Sigma = (n^2 + 1^2) = 5$ boundary, the same one as above