CSL Boundaries

1. what do we need to define grain boundary??
2. CSL geometry
3. Measuring orientations of CSL
4. CSL Model
5. Grain boundaries properties
6. Effect of CSL on Mechanical property
7. Grain Size vs CSL
8. Factors influencing the Proportion of OF CSL boundaries
9. Recrystallisation and CSL
10. Effect of CSL on Creep,Superplasticity
11. Limitations
12. Conclusion

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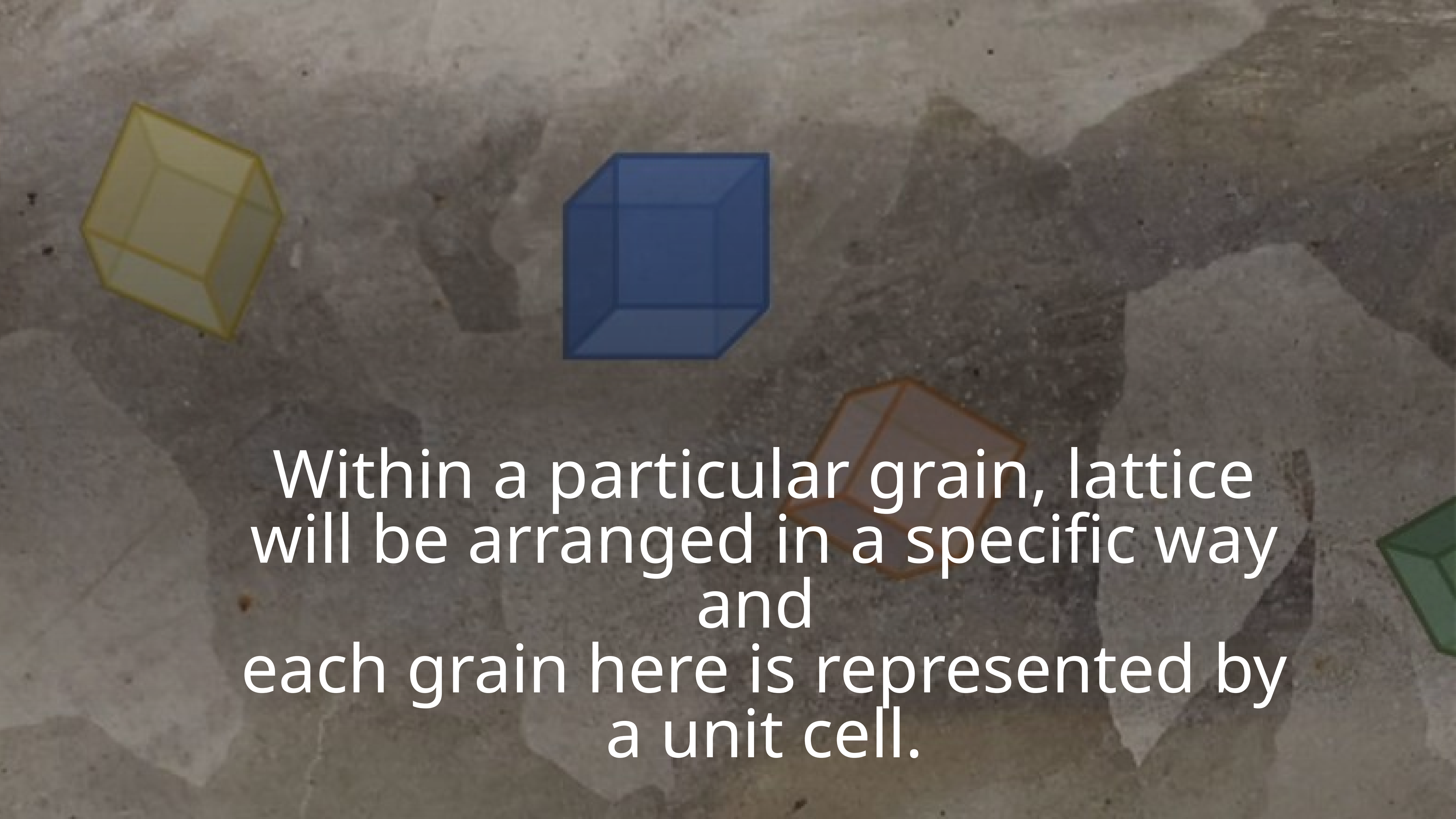
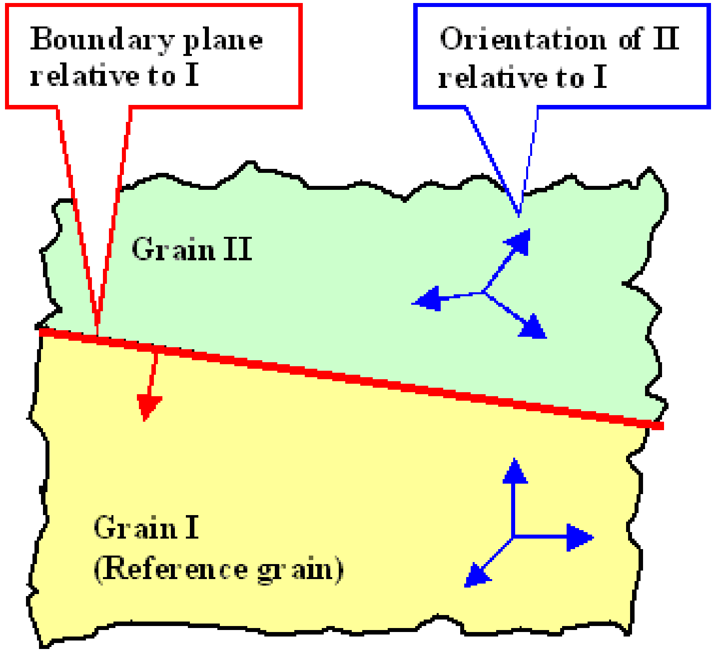
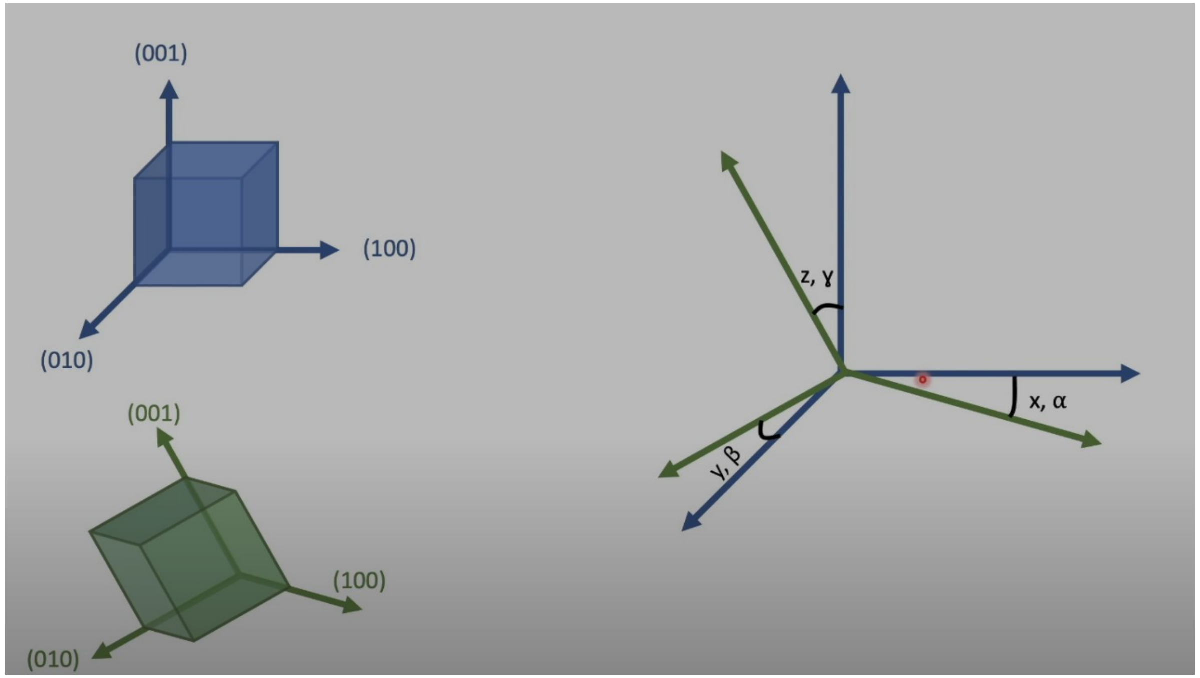
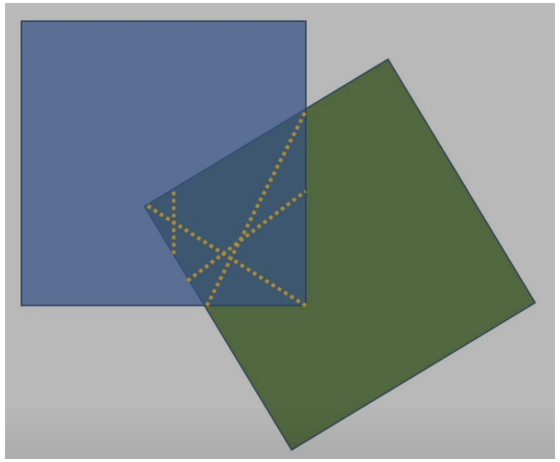

Within a particular grain, lattice
will be arranged in a specific way
and
each grain here is represented by
a unit cell.

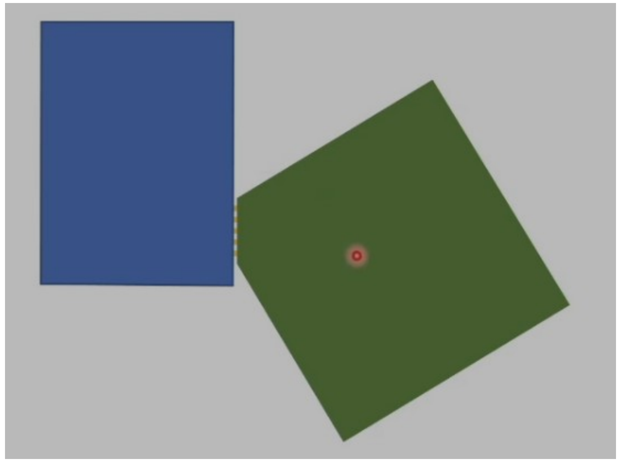
- Just knowing the orientation is not going to help we need to define it quantitively
- We choose a reference axis and define angle with respect to that reference axis.
- This will give the misorientation of grain II with respect to grain I—(not enough to define the grain boundary) what we need to define is the grain boundary plain.

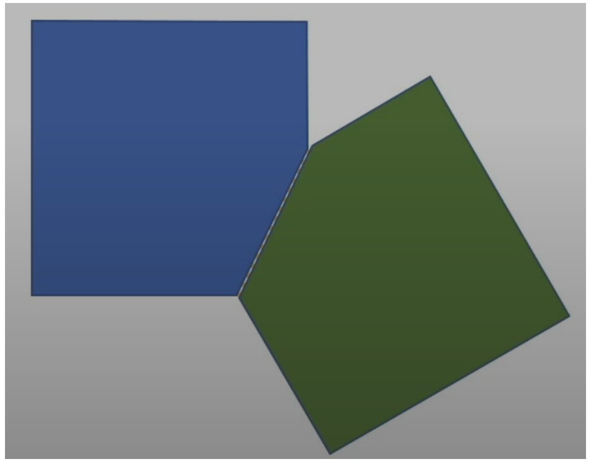




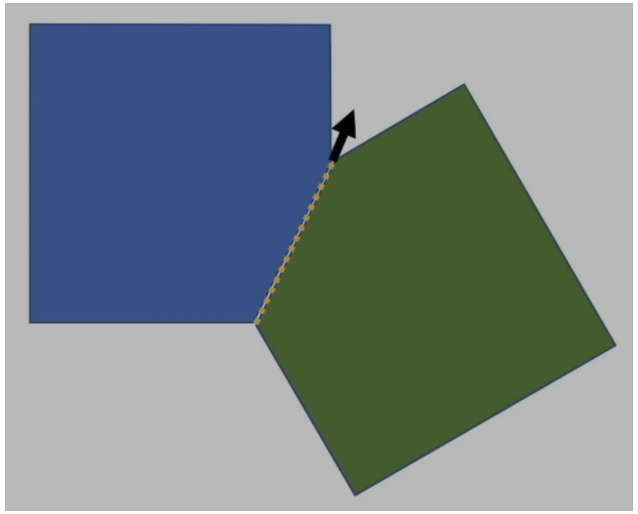
- In order to define GB plane we can cut it on any plane mentioned below(orientation is fixed) below is the two mentioned along two different plane that will result in a grain boundary
- This means while growing they met along that particular plane
- h^2 + k^2 +l^2 = 1, where h, k and l are unit vector.
- In total we have this 5 macroscopic degrees of freedom to define a grain boundary which contain 3 angles representing orientation and wo parameters to define the boundary plane by its Miller indices {hkl}

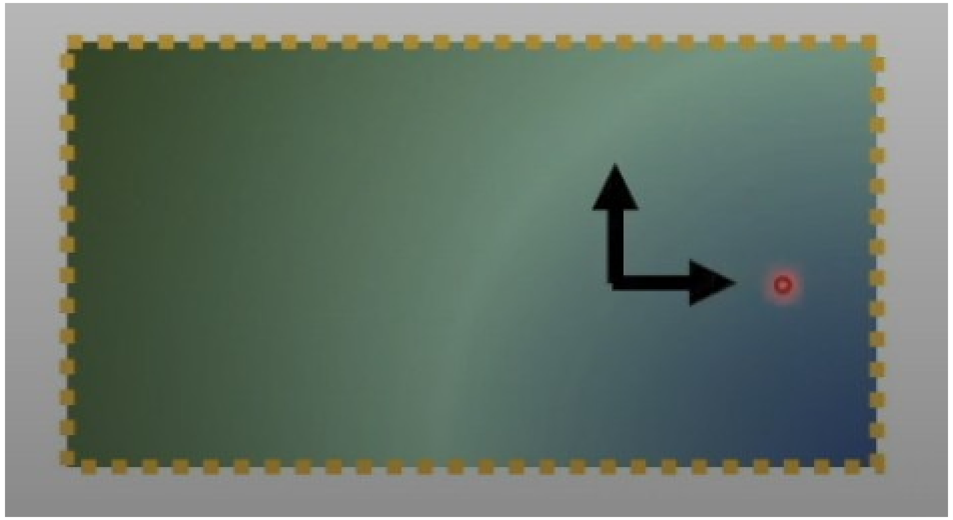




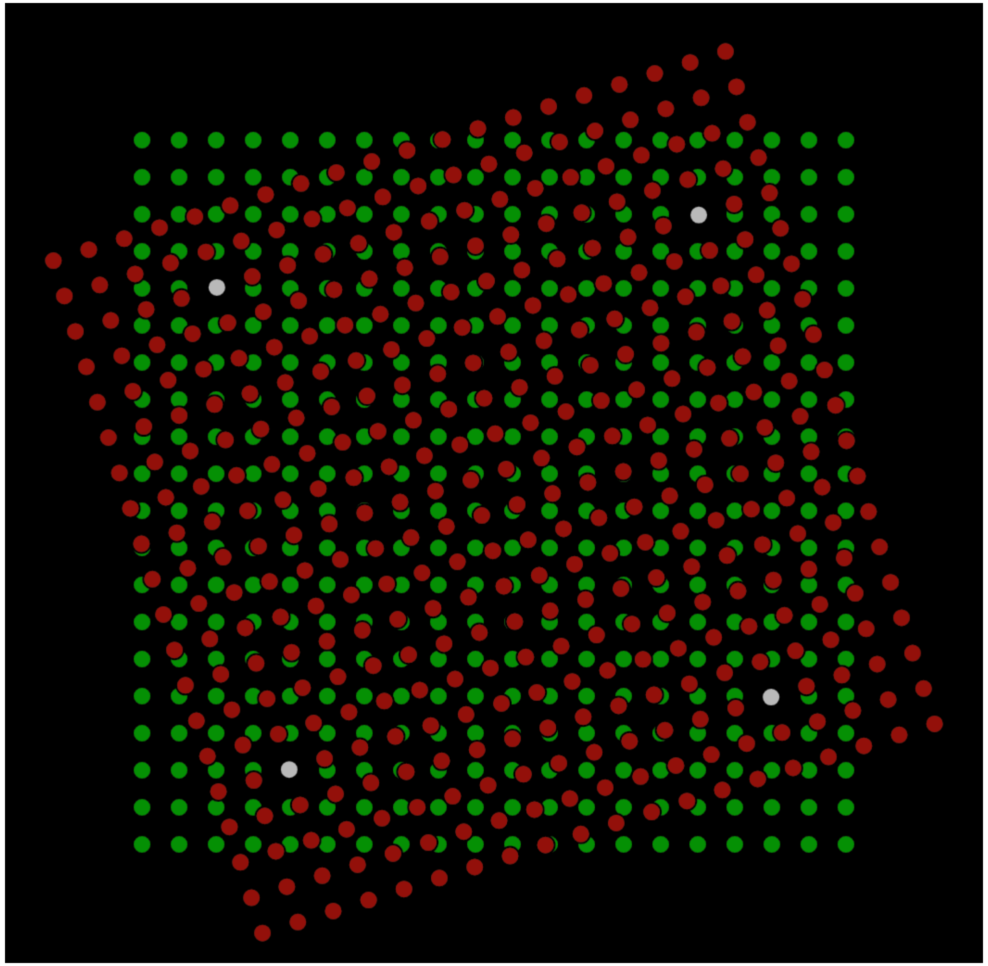


- 3 additional microscopic degree of freedom for a grain boundary-GB plane can slide along the plane and perpendicular to the plane.



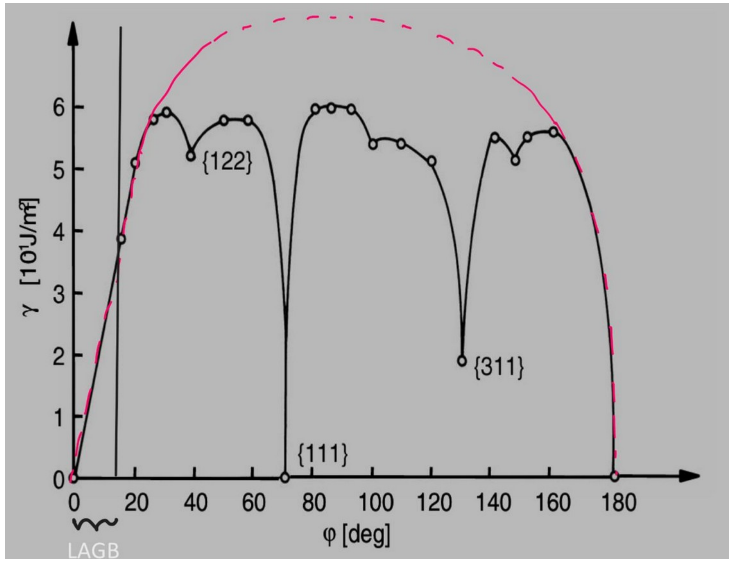


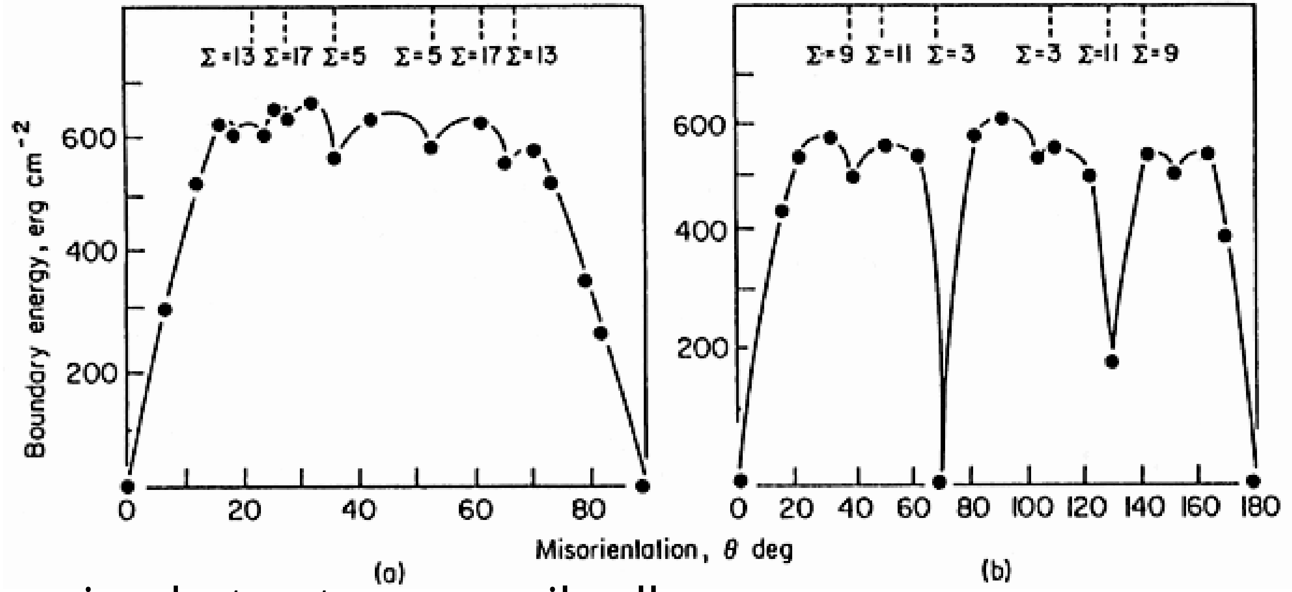
Geometry of CSLs Grain Boundary



https://editor.p5js.org/ashishb230198/sketches/wLvZ65pau

- Low Σ boundaries tend to have lower energies than average???
- However increase in energy is not monotonic with with increasing Σ!, There might be some Σ values with especially low energy values, whereas others are not very special if compared to a random orientation.
- The result of (simple) calculations for special cubic geometries are shown in the picture:
- We see that the energies are lower, indeed, in low Σ orientations, but that it is hard to assign precise numbers or trends(shown Images Al produced by rotating around a <100> axis (left) or a <110> axis (right) at 0 k)





Clearly, some Σ boundaries have low energies, but not necessarily all.

Image is taken from: https://www.tf.uni-kiel.de/matwis/amat/def_en/kap_7/backbone/r7_1_2.html

- A so-called Moiree pattern develops and for certain angles some lattice points of lattice 1 coincide exactly with some lattice points of lattice 2. A kind of superstructure, a coincidence site lattice (CSL), develops.

- Many coincidence relations exist for two identical two-dimensional lattices. In order to be able to extend the **CSL** consideration to three dimensions and to generalize it, we have to classify the various possibilities

Definition:
The relation between the number of lattice points in the unit cell of a **CSL** and the number of lattice points in a unit cell of the generating lattice is called Σ (Sigma); it is the unit cell volume of the **CSL** in units of the unit cell volume of the elementary cells of the crystals.

$$\Sigma = \frac{\text{volume elementary cell of CSL}}{\text{volume elementary cell of crystal lattice}}$$

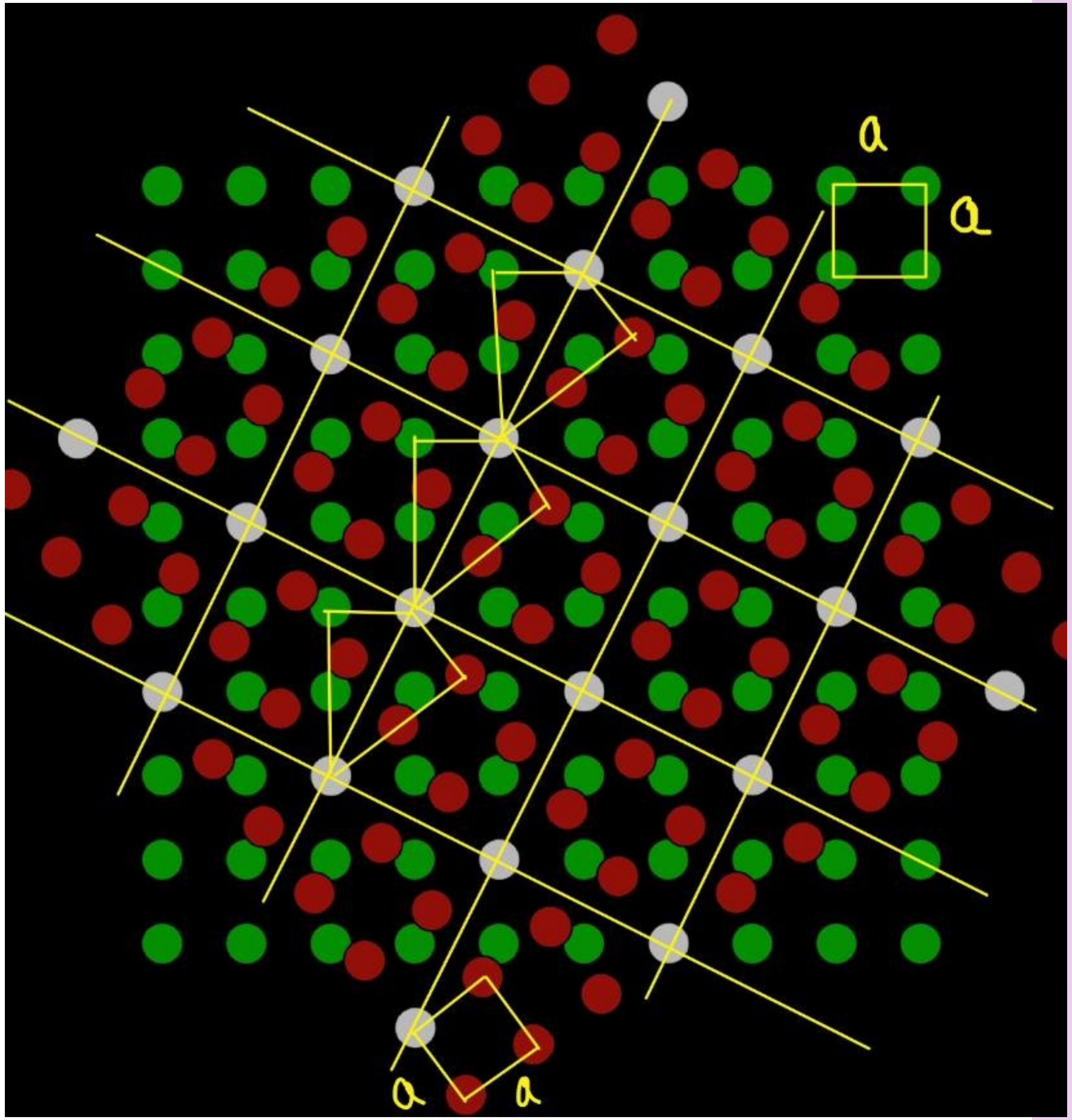
- Since both crystal lattices are periodic, the coincidence sites also must be periodic, i.e. they also define a lattice, the coincidence site lattice (CSL).

- For the rotation 36.87◦ <100> is Σ = a(a√5)2/ a3 =5

- A Σ1 boundary thus would denote a perfect (or nearly perfect) crystal; i.e. no boundary at all.

- Since the numerical value of Σ is always odd, the twin boundary is the grain boundary with the most special coincidence orientation there is, i.e. with the largest number of coinciding lattice points.

- That grain boundaries between grains in a CSL orientation, especially if the Σ values are low, have particularly small grain boundary energies.

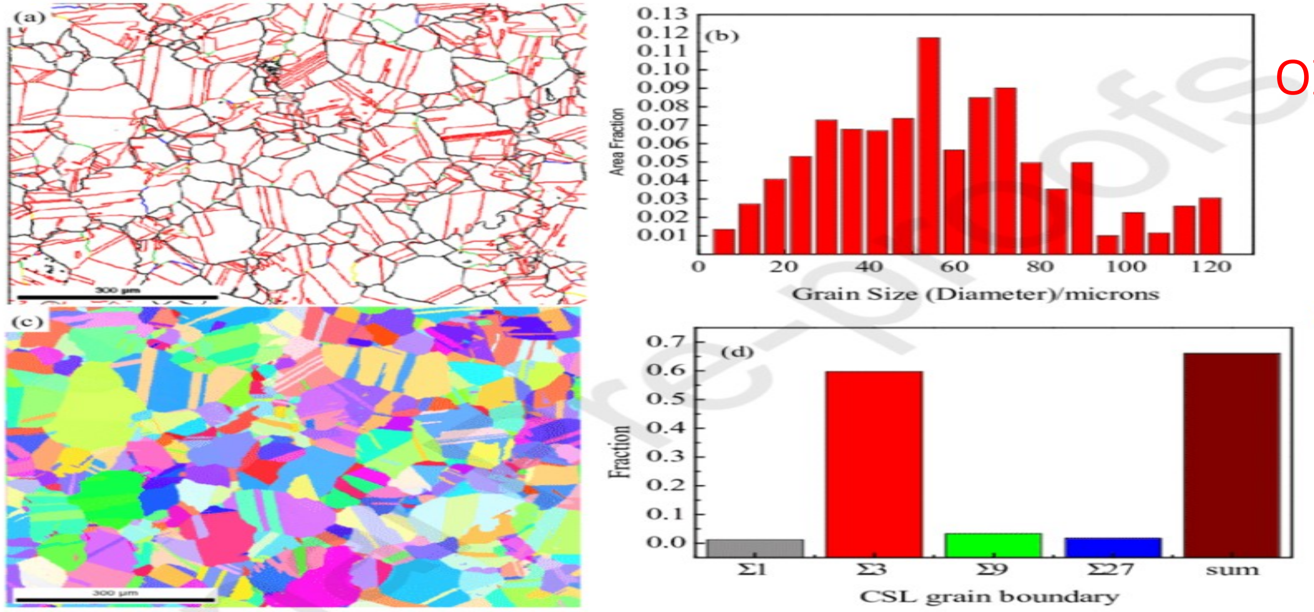


Measuring orientations of CSL

- Many imaging techniques such as EBSD,TEM,Orientation imaging analysis can be employed to analyze the orientations of CSL boundaries.

- Which one do you prefer and why?

- Well you can also analyze Kikuchi patterns in a TEM to obtain orientation relationships but preparation of specimen is time consuming.



OIM OF CSL BOUNDARIES

Figures is taken from: https://www.researchgate.net/figure/a-OIM-image-b-grain-size-distribution-c-orientation-distribution-of-the-grains-and_fig1_349402484

CSL MODEL

- CSL model is just a geometric model that accounts for the special properties exhibited due to abnormal low energies of the boundary planes
- However the model did not appeal to majority of the contemporaries since it was published.
- The reason being is the unknown myth in relating just a geometric model to special properties where other factors such as chemical interactions etc must also be considered.

ONTARIO HYDRO COMPANY

- At Ontario hydro, processing technologies for grain boundary engineered wrought austenic steels and high performance nickel alloys have been incorporated into production with atmost 60% proportion of special boundaries.
- With this technology , they were able to enhance increased protection against intergranular corrosion,stress corrosion ,cracking

Grain boundary properties

- There are properties that are directly linked to the geometry of the grain boundaries.
- Those are termed as intrinsic grain boundary parameters.

1. ENERGY
2. SEGGREGATION
3. DIFFUSIVITY
4. MOBILITY OR MIGARTION
5. RESISTIVITY

- These parameters are dependent directly on the amount of free volume in the boundary plane.(HOW?)

- Some tilt and twist boundaries, i.e. CSLs having particular boundary planes, are characterised by a lower than average free volume and therefore are associated with property values which differ from the average.

THE ROLE OF CSL BOUNDARIES IN MECHANICAL BEHAVIOUR OF MATERIALS

- Failure of materials is atmost a cause of intergranular degradation i.e formation of cavities, fracture, corrosion and embrittlement etc and low energy boundaries are also those which are resistant to intergranular degradation.

- All the above phenomena show sharp discontinuities in values for special boundaries, Therefore special boundaries are of more interest to study.

- From the experimental verifications, it was found that these CSL boundaries with minimal energy are always resistant to intergranular degradation.

- Usually to minimize their energy and attain stability, grain boundaries often undergoes the following phenomena:

  1. Annealing twinning
  2. Grain boundary recovery
  3. Grain rotation
  4. Grain growth

GRAIN SIZE VS CSL

- Usually we examine a set of csl boundaries by setting their maximum value to 29 or 49 and investigate further to know about the properties. (WHY?)
- There is no universal rule that small grain boundaries contribute to higher proportion of csl boundaries. But evidences from experiments suggests it.

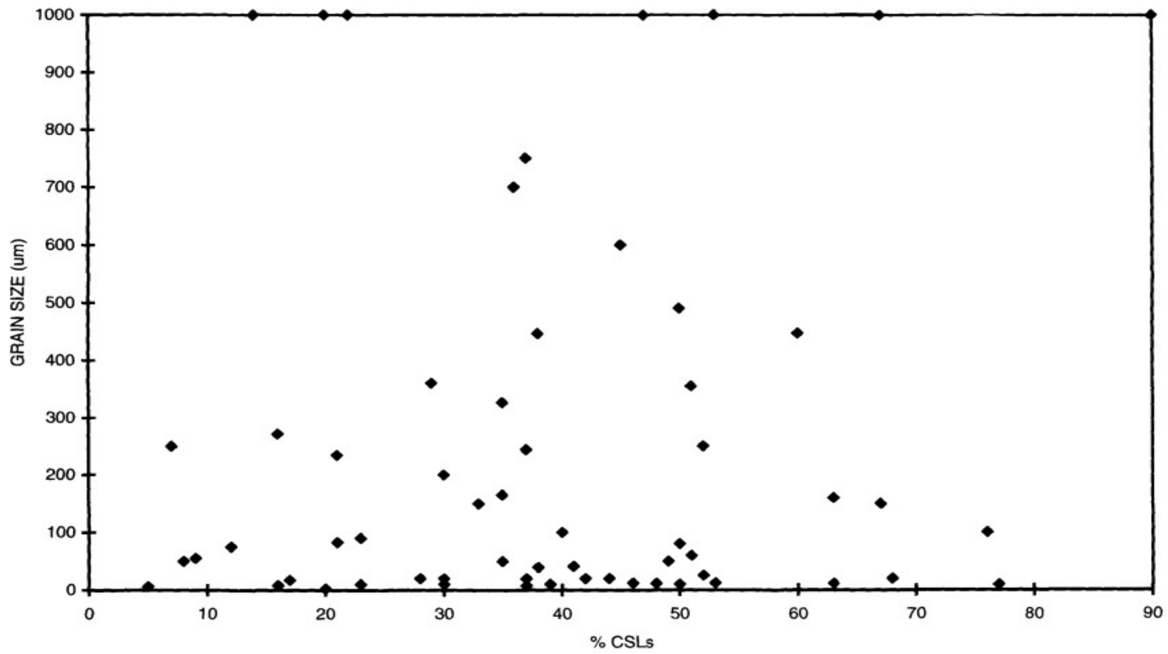


Figure is taken from: The Role of the Coincidence Site Lattice in Grain Boundary Engineering by Valerie Randle

FACTORS THAT INFLUENCE THE PROPORTION OF CSL BOUNDARIES:

- THE PRESENCE OF STRONG TEXTURE, RESULTING IN THE FORMATION OF SIGMA 1 BOUNDARIES

- THE AMOUNT OF TWINNING THAT RESULTS IN THE FORMATION OF SIGMA 3 AND SIGMA 3**N BOUNDARIES

- MOST OF THE BCC ELEMENTS AND ALUMINIUM(EXCEPTION) ARE MORE SUSCEPTIBLE TO THE FORMATION OF SIGMA 1 BOUNDARIES.

- SIMILARLY FCC METALS AND ALLOYS SUCH AS COPPER,NICKEL,THEIR ALLOYS AND AUSTENIC STEELS ARE MORE SUSCEPTIBLE TO THE FORMATION OF SIGMA 3 BOUNDARIES.

- THE SAME PROPORTION OF CSLs IN DIFFERENT MATERIALS GIVE DISTINCT DISTRIBUTION PROFILES.

Material	SFE (mJm^{-2})	$\%\Sigma 3$
Al	170	5
Ni	130	28
Cu	80	45

Table is taken from: The Role of the Coincidence Site Lattice in Grain Boundary Engineering by Valerie Randle

RECRYSTALLISATION AND CSL

- CSL boundaries play a prominent role in forming a texture during the process of recrystallisation

- Grain boundary migration is the phenomena involved in the process of recrystallisation. Usually HAGBs possess greater grain mobility. (Is it always the case? Think of sigma 7 boundaries in recrystallisation of Al)

- CSL offer a barrier to grain boundary migration that help in maintaining texture, and secondary recrystallisation is also possible with the selective grain growth.(discussed in next slide)

- Hence, for example, a typical rolling texture, (011)(211), and recrystallisation texture, (311) [112], for austenitic steels is related by a misorientation which is close to sigma 29 boundary.

- The consequence of the lack of exactness in many CSLs ascribed to orientation relationships across recrystallisation interfaces is that they cannot be linked rigorously to special properties

SECONDARY RECRYSTALLISATION IN SI-FE ALLOY

- There is a direct technological interest, for Fe—3%Si transformer steels, in the growth of very large grains having the so-called 'Goss texture', (110)[001], This is essential in obtaining the optimum magnetic properties.
- As discussed earlier, CSL inhibit the grain boundary migration maintaining texture without growing in random direction and grain growth occurs in only certain selective grain boundaries where the absence of CSLs is noted.
- It can be predicted by "SIMULATION BY HYPOTHETICAL NUCLEUS METHOD"
- DO all CSLs inhibit the grain boundary mobility? .

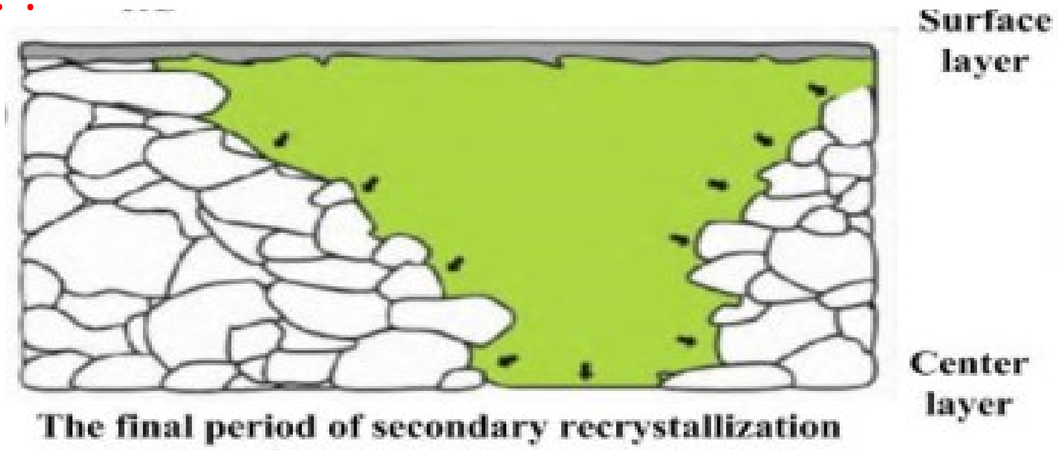


Image is taken from: https://www.mdpi.com/2073-4352/13/9/1396

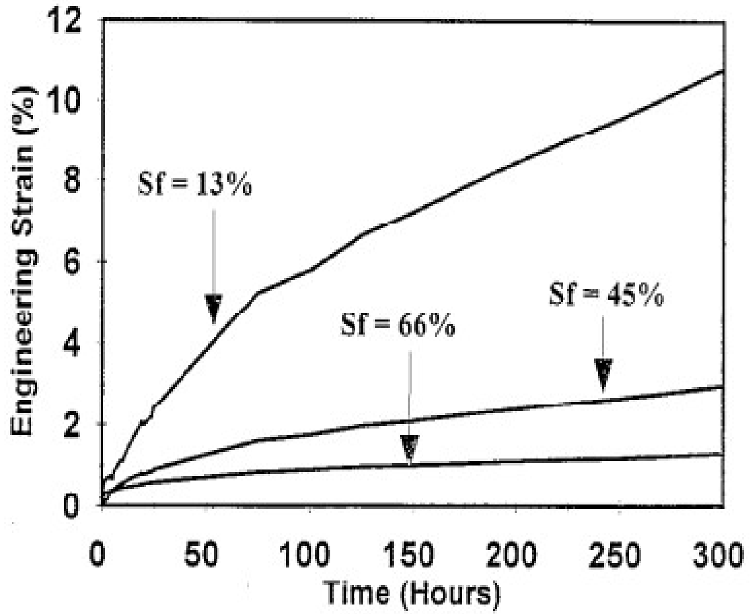
EFFECT OF CSL ON CREEP

Creep rate can be minimized by increasing the proportion of sigma 3 boundaries.

Table 1
Comparison of the grain boundary character distribution in cast versus two wrought (processed) 99.99% nickel samples

Boundary type Σ	Boundary frequency (%)		
	Cast (GS = 50 μm)	Wrought #1 (GS = 35 μm)	Wrought #2 (GS = 25 μm)
1	4.0	6.6	8.0
3	1.6	27.9	46.7
5	0.9	0.6	0.2
7	0.7	0.6	0.5
9	1.3	3.9	5.5
11	0.3	0.4	0.7
13	1.0	0.7	0.5
15	0.2	0.6	0.5
17	0.3	0.2	0.1
19	0.3	0.5	0.7
21	0.7	0.3	0.2
23	0.6	0.3	0.1
25	0.4	0.4	0.1
27	0.8	1.8	2.2
29	0	0.3	0.1
> 29 (Random)	86.9	54.9	35.8
Total Σ ≤ 29 'special' fraction (%)	13.1	45.1	66.2

GS, grain size.



https://www.sciencedirect.com/science/article/pii/S0921509397001263

EFFECT OF CSL ON SUPERPLASTICITY

- Grain boundary sliding is the mechanism involved in raising superplasticity.
- It is usually achieved at high temperatures with fine grain size.
- High angle grain boundaries thus promote the grain boundary migration strongly, therefore minimizing CSL proportion is shown to increase superplasticity.
- Think of processing techniques to minimize the proportion of CSLS?(AREA OF RESEARCH)

LIMITATIONS

- Most of our results are a direct verifications from the experiments performed on synthesised BICRYSTALS.
- However, extending the concept to polycrystals is a challenging and on going research field. (only Ontario hydro company was successful in it)
- Yet there were no extensions of CSL theory to intermetallics and superconductors.(a big interest in material science field)
- Challenge: Do research and apply CSL concept to superconductors and synthesize any material that behaves as superconductor at any temperature? THIS WILL REVOLUTIONIZE THE WHOLE WORLD.

CONCLUSIONS

- CSL boundaries are special boundaries that exists with unique misorientions where abnormal low energies are observed than excepted.
- Due to their abnormal low energy, many mechanical properties such as corrosion, strength, creep, superplasticity etc are influenced by them greatly.
- CSL boundaries offer a great resistance to intergranular degradation and corrosion. Creep resistance is increased by increasing proportion of csl boundaries.
- Superplasticity is achieved at high temperature with fine grain size by limiting the csl proportion too low.
- Preferred growth in certain orientations such as gauss orientation by secondary recrystallization to obtain the optimum magnetic properties in Fe-3%Si alloy transformers.
- Processing techniques to enhance the proportion of CSLs is still a research field.

REFERENCES

1. K.T. Aust and J.W. Rutter, Trans. TMS-A1ME 215 (1959) 119.
2. G. Herrmann, H. Gleiter and G. Baro, Acta Metall. 24 (1976) 353.
3. A.P. Sutton and R.W. Baluffi, Acta Metall. 35 (1987) 2177.
4. L Priester, Revue Phys. Appl. 24 (1989) 419.
5. S.CM.L. Kronberg and F.H. Wilson, Met. Trans. 185 (1949) 501.
6. Mehta and D.A. Smith, Proc. Grain boundary engineering, Ed. U. Erb and G. Palumbo, Canadian. Inst. Min., Met. & Petrol, Montreal (1994) 89.
7. P.J. Goodhew and D.A. Smith, Scripta Met. 14 (1980) 59.
8. R.A. Varin, Phys. Stat. Sol. 51A (1979) kl89.
9. L.S. Shvindlerman and B.B. Straumal, Acta Metall. 33 (1985) 1735.
10. https://youtu.be/QaBQirHXvtE?si=uYLZABU2Cy2FmAAx
11. https://www.tf.uni-kiel.de/matwis/amat/def_en/kap_7/backbone/r7_1_2.html
12. https://youtu.be/IFMdrlOtS4k?si=0FHwUurH9hk8VUpY

Book we preferred..

- The Role of the Coincidence Site Lattice in Grain Boundary Engineering by Valerie Randle