EPFL
École polytechnique fédérale de Lausanne

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SuNMiL
Supramolecular NanoMaterials and Interfaces Laboratory

Solid-Solid Interfaces
Lesson 8

MSE 304

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Key Topics in the Previous Class

$$\gamma_{\alpha\beta} = \gamma_{\alpha} + \gamma_{\beta} - W_{\alpha\beta}$$

fluid - fluid → diffuse interfaces

Reading for this Class

Chapter 13 Howe book

L: very little

L: all of it

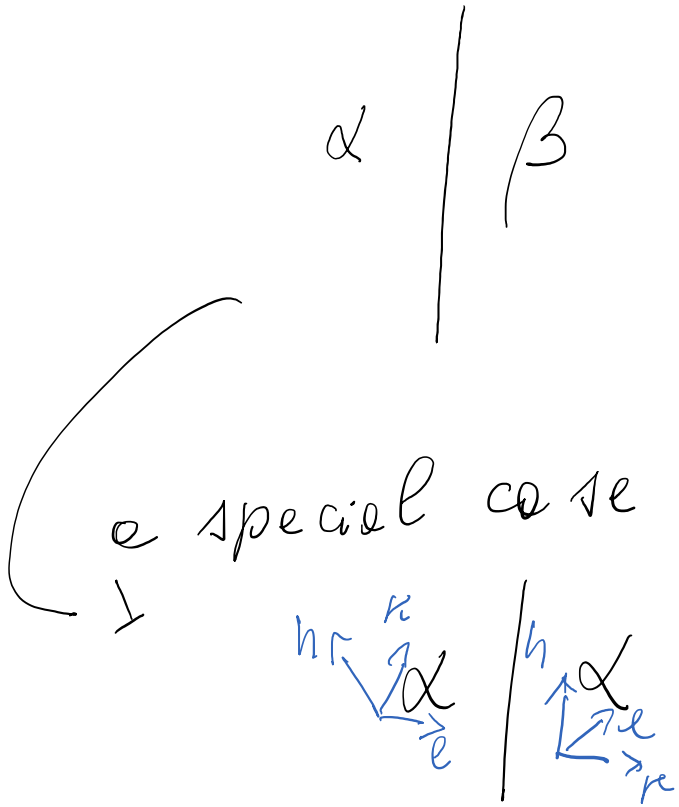
Questions to be answered in Class

1) Is the TLK model compatible with a simple Langmuir model?

i molecule can form a monolayer

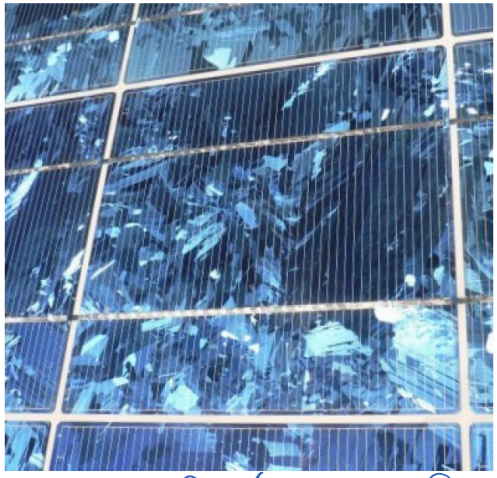
2) ~~or~~ does it always form micelle in a fluid phase & if the concentration exceeds the CMC?

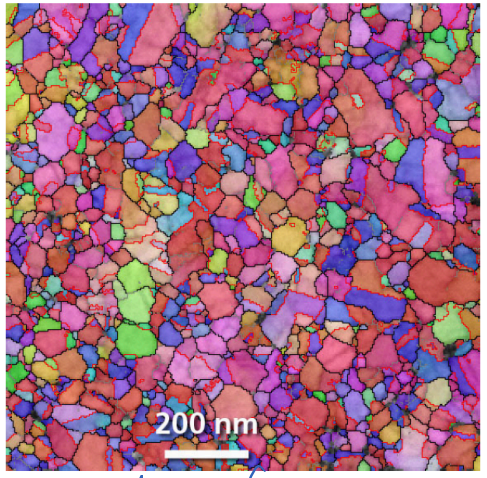
Solid-Solid Interfaces



Solid-Solid Interfaces

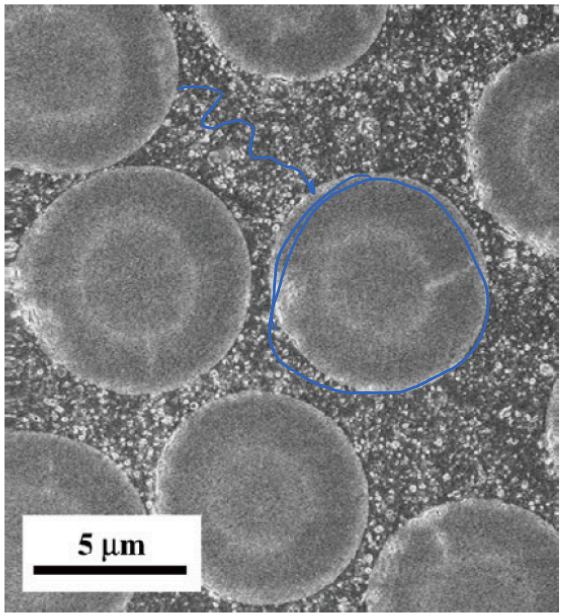
- Most bulk materials are polycrystalline, composed of many grains with different orientation
  - Grain boundaries affect mechanical or electronic properties
  - The story gets even more complex when it comes to interfaces between different phases (heterophase interfaces)

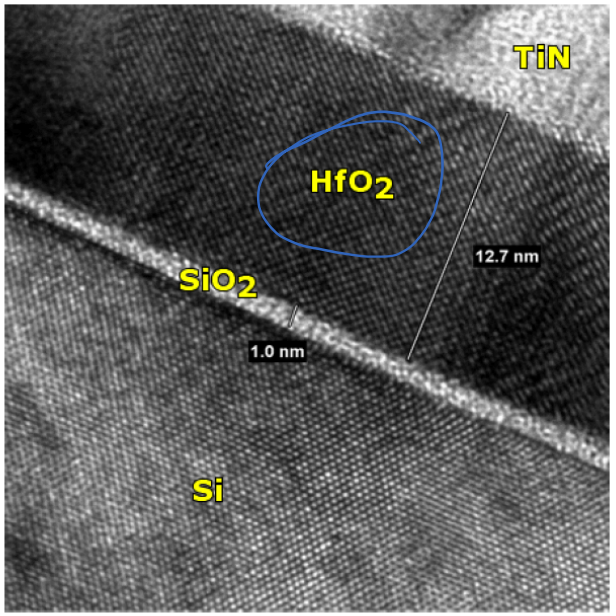




Grain boundary is a solid-solid interface

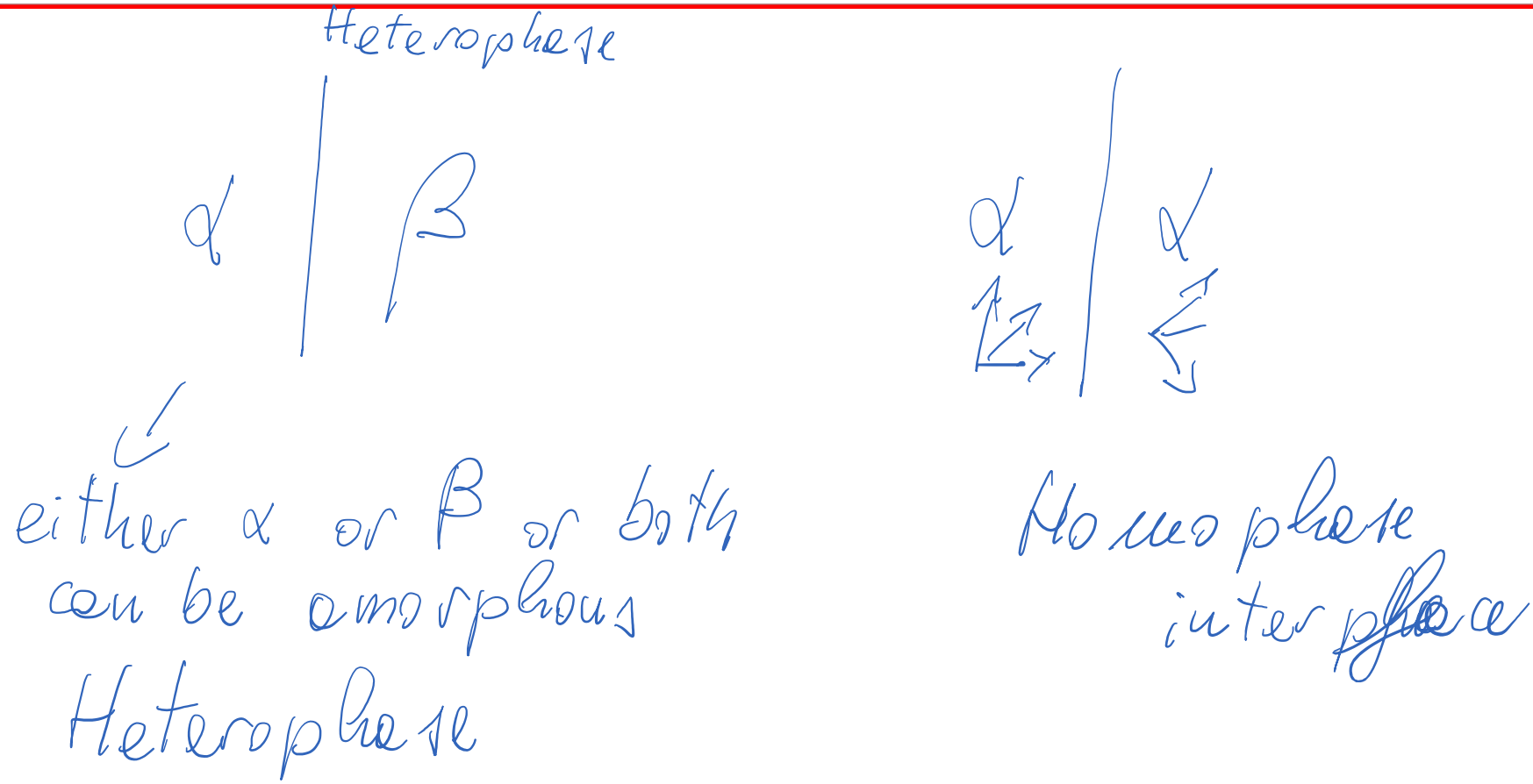
Solid-Solid Interfaces





Grain boundary engineering is key to determine mechanical and electronic properties

Homophase and ~~Eteropahse~~ Solid-Solid Interfaces



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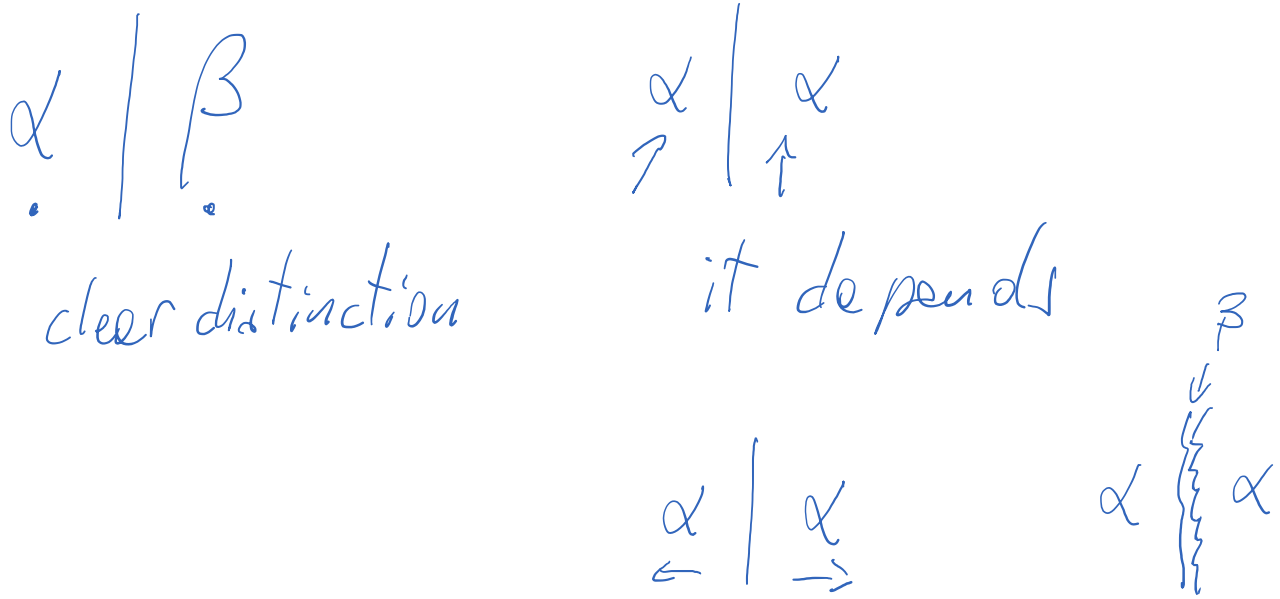
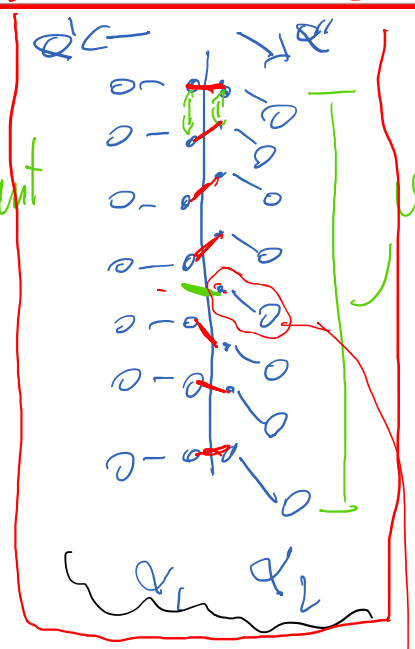
Homophase and Heterophase Solid-Solid Interfaces



Homophase Solid-Solid Interfaces



Why b is different for α_1 and α_2

unit area

$$\gamma_{\alpha_1\alpha_2} = \gamma_{\alpha_1} + \gamma_{\alpha_2} - W_{\alpha_1\alpha_2}$$

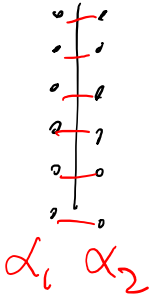
break break reform

?

→ energy of a single bond broken plus the elastic energy to stretch all the red reformed bonds past their equilibrium length

Solid-Solid Interfaces

$$\lim_{\theta \to 0} \gamma_{\alpha_1 \alpha_2} = \gamma_{\alpha_1} + \gamma_{\alpha_2} - W_{\alpha_1 \alpha_1} = 0$$



$$W_{\alpha_1 \alpha_1} = 2\gamma_{\alpha_1} \quad \left(\lim_{\theta \to 0}\right)$$

a few dangling bond + ↑ plus elastic energy

homophase solid surfaces → $W_{\alpha_1 \alpha_2} \simeq \gamma_{\alpha_1} + \gamma_{\alpha_2}$

Solid-Solid Interfaces

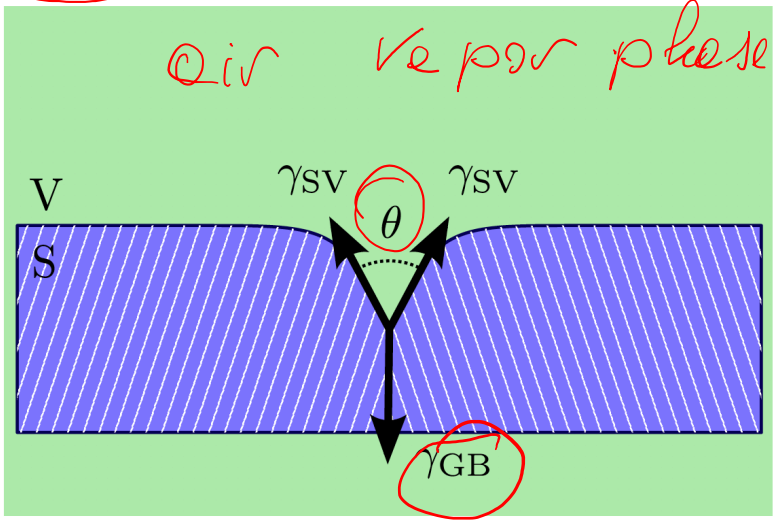
- One can associate a surface-energy term γ_{GB} to the presence of GBs

$$\gamma_{GB} = 2\gamma_{SV} - W_{GB}$$

  - The GB energy can be estimated by thermal grooving
  - Balance between surface energy γ_{SV} and γ_{GB} (typically $\gamma_{SV} \approx 3\gamma_{GB}$)

$$2\gamma_{SV}\cos\frac{\theta}{2} = \gamma_{GB}$$

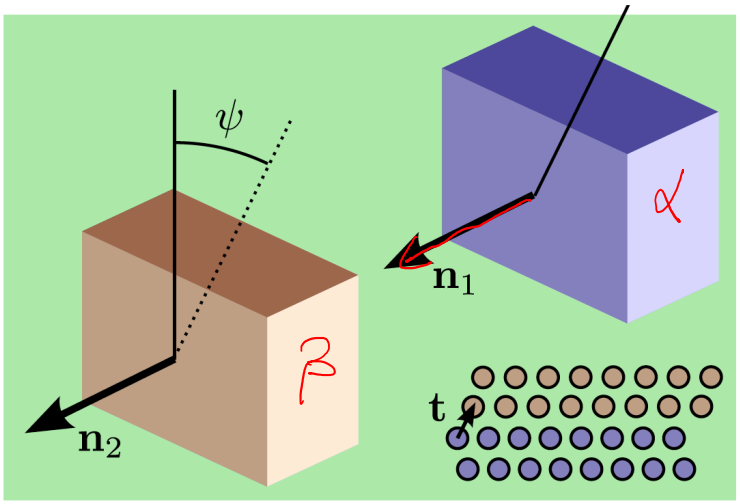
- What happens if $\gamma_{GB} > 2\gamma_{SL}$?



Solid-Solid Interfaces

for your consideration

- How many parameters we need to describe the geometry of a GB?
  - Orientation of the two surfaces + relative tilt = 5 degrees of freedom
  - Atomic-scale register between the surfaces
- Simpler geometry - simmetric tilt boundaries



β could be α_2

5 degrees of freedom between $\vec{n}_1$ and $\vec{n}_2$

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Conclusions

$$\gamma_{\alpha\beta} = \gamma_\alpha + \gamma_\beta - W_{\alpha\beta}$$

$$W_{\alpha\beta} \simeq \gamma_\alpha + \gamma_\beta$$

count interfacial dislocations

or

compute interfacial (elastic) stress

or

both