Self-consistent scheme

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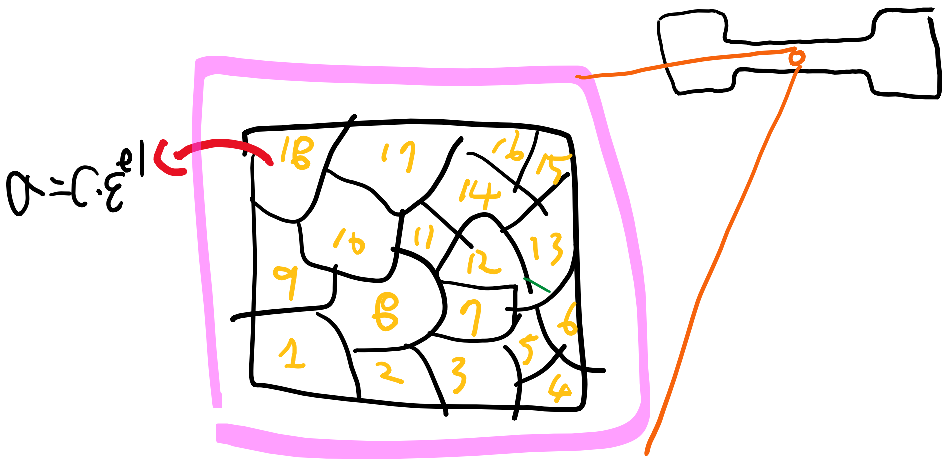
The entire response/stimulus and individual response/stimulus?



가정 (앞으로 이어질 논의의 이해를 돕기 위한 세가지 가정을 도입하자)

- 각 grain의 moduli(혹은 compliance)가 알려져 있다.
- 각 grain내의 stress, strain 반응은 uniform (즉 위치에 따라 달라지지 않는다)
- 각 grain들의 weight가 동일

* These are not "REQUIRED", but will make our analyses simple.

Reminding our goal:

- Our goal is to find the property of entire aggregate using the property of each member.

가령 $\mathbb{M}^{el}$ 를 사용해서 $\bar{\mathbb{M}}^{el}$ 를 알아내기.

가령 $\mathbb{C}^{el}$ 를 사용해서 $\bar{\mathbb{M}}^{el}$ 를 알아내기.

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아마 각 grain의 성질의 평균값을 사용하면 될 것 같은데?

가령 $\mathbb{M}^{el}$ 를 사용해서 $\bar{\mathbb{M}}^{el}$ 를 알아내기.

$$\bar{\mathbb{M}}^{el} = \frac{\mathbb{M}^{el,\text{grain \#1}} + \mathbb{M}^{el,\text{grain \#2}} + \dots + \mathbb{M}^{el,\text{grain \#n}}}{\text{n}}$$

weighted average.

$$\bar{\mathbb{M}}^{el} = \frac{\mathbb{M}^{el,\text{grain \#1}} \cdot w^{\text{grain \#1}} + \mathbb{M}^{el,\text{grain \#2}} \cdot w^{\text{grain \#2}} + \dots + \mathbb{M}^{el,\text{grain \#n}} \cdot w^{\text{grain \#n}}}{w^{\text{grain \#1}} + w^{\text{grain \#2}} + \dots + w^{\text{grain \#n}}}$$

$$= \mathbb{M}^{el,\text{grain \#1}} \cdot f^{\text{grain \#1}} + \mathbb{M}^{el,\text{grain \#2}} \cdot f^{\text{grain \#2}} + \dots + \mathbb{M}^{el,\text{grain \#n}} \cdot f^{\text{grain \#n}}$$

Fraction: $f^i = \frac{w^i}{\sum_i w^i}$

$$\bar{\mathbb{M}}^{el} = \langle \mathbb{M}^{el} \rangle$$

weighted average in short form.

We will focus on two extreme cases first

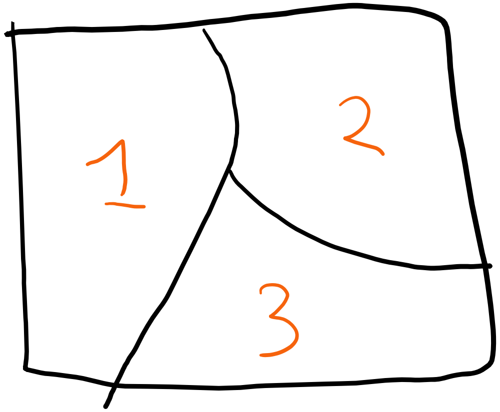
Case 1: $\bar{\mathbb{C}}^{el} = \langle \mathbb{C}^{el} \rangle$

Thus, $\bar{\mathbb{M}}^{el} = \left(\bar{\mathbb{C}}^{el}\right)^{-1}$

Case 2: $\bar{\mathbb{M}}^{el} = \langle \mathbb{M}^{el} \rangle$

* The above two cases may lead to "equivalent" results OR NOT!

Grain이 3개로 구성된 aggregate를 대상으로 살펴보자.



$$f^1 = \frac{1}{3}$$

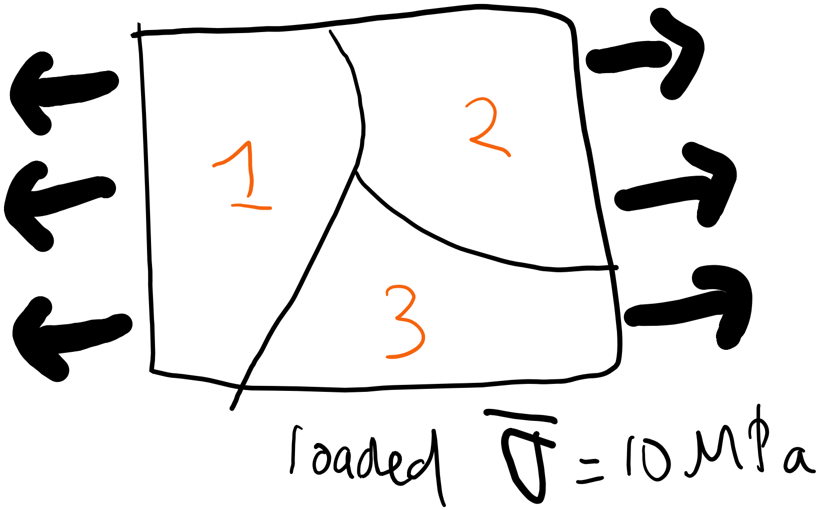
$$f^2 = \frac{1}{3}$$

$$f^3 = \frac{1}{3}$$

각 grain들이 다 같은 weight fraction을 가진 것으로 가정했다.

우리가 다루는 3개의 grain으로 구성된 polycrystal이 매우 부적절해 보일 수 있으나, 이를 바탕으로 얻어낸 결과들은 weight fraction이 서로 다른 polycrystal에도 동일하게 적용이 가능하다. 따라서 이러한 간단한 케이스부터 다루는 것이 쉽고 유용하다.

Case 1.



$f^1 = \frac{1}{3}$

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$f^3 = \frac{1}{3}$

만약 다결정이 전체적으로 $\bar{\sigma} = 10\ [MPa]$ 만큼의 응력이 받는다면, 얼마만큼의 탄성 변형량($\bar{\varepsilon}^{el}$)을 보일까?

what is $\bar{\varepsilon}^{el}$?

각 grain의 moduli: $\mathbb{C}^{el} = 200\ [GPa]$ 로 주어졌다.

각 grain의 성질 $\mathbb{C}^{el}$ 은 주어졌지만, 전체 다결정의 성질 $\bar{\mathbb{C}}^{el}$은 주어지지 않았다. 다결정의 $\bar{\varepsilon}^{el} = \bar{\mathbb{M}}^{el}\bar{\sigma}$ 구성방정식을 통해 탄성 변형량을 알기 위해서는 다결정의 성질 (compliance of polycrystal) $\bar{\mathbb{M}}^{el}$ 을 알아야 한다.

If we apply the 1st extreme cases

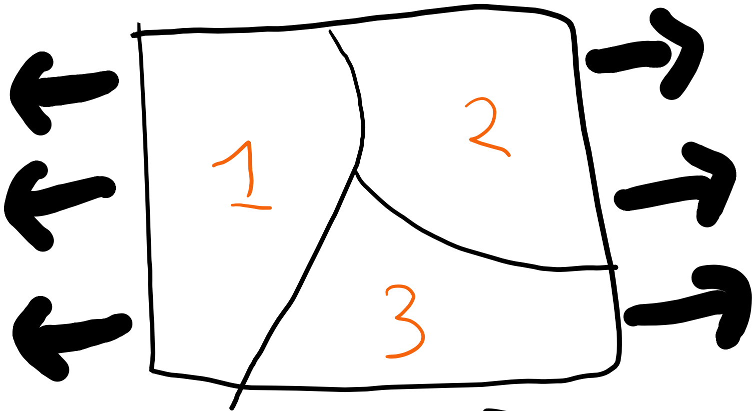
$$\bar{C}^{el} = \langle C^{el} \rangle = \sum_{i}^{3} C^{el,i} \times f^{i} = 200 \times \frac{1}{3} + 200 \times \frac{1}{3} + 200 \times \frac{1}{3}$$

$$= 200\ [GPa]$$

$$\bar{M}^{el} = (\bar{C}^{el})^{-1} = \frac{1}{200}\ [GPa^{-1}]$$; Elastic compliance

$$\bar{\varepsilon}^{el} = \bar{M}^{el} \cdot \bar{\sigma} \longrightarrow \bar{\varepsilon}^{el} = \frac{1}{200} \frac{1}{[GPa]} \times 10\,[MPa] = 5 \times 10^{-5}$$

Case 2.



loaded $\bar{\sigma} = 10\,MPa$

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만약 다결정이 전체적으로 $\bar{\sigma} = 10\ [MPa]$ 만큼의 응력이 받는다면, 얼마만큼의 탄성 변형량($\bar{\varepsilon}^{el}$)을 보일까?

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$\rightarrow M^{el} = (\mathbb{C}^{el})^{-1} = \frac{1}{200\,[GPa]}$

각 grain의 성질 $\mathbb{C}^{el}$ 은 주어졌지만, 전체 다결정의 성질 $\bar{\mathbb{C}}^{el}$은 주어지지 않았다. 다결정의 $\bar{\varepsilon}^{el} = \bar{\mathbb{M}}^{el}\bar{\sigma}$ 구성방정식을 통해 탄성 변형량을 알기 위해서는 다결정의 성질 (compliance of polycrystal) $\bar{\mathbb{M}}^{el}$ 을 알아야 한다.

If we apply the 2nd extreme cases

$$\bar{M}^{el} = \langle M^{el} \rangle = \sum_{i}^{3} M^{el,i} \times f^i = \frac{1}{200} \times \frac{1}{3} + \frac{1}{200} \times \frac{1}{3} + \frac{1}{200} \times \frac{1}{3}$$

$$= \frac{1}{200}\,[GPa^{-1}]$$

Elastic compliance

$$\bar{\varepsilon}^{el} = \bar{M}^{el} \cdot \bar{\sigma} \longrightarrow \bar{\varepsilon}^{el} = \frac{1}{200}\frac{1}{[GPa]} \times 10\,[MPa] =$$

Conclusions from Cases 1 and 2.

1. $\bar{C}^{el} = \langle C^{el} \rangle$

   Thus, $\bar{M}^{el} = \left(\bar{C}^{el}\right)^{-1}$; inverse

2. $\bar{M}^{el} = \langle M^{el} \rangle$

   Thus, $\bar{C}^{el} = \left(\bar{M}^{el}\right)^{-1}$

The two extreme cases 1 & 2

led to the same results.

Summary

- What we have assumed:
  - We have tacitly assumed that the quantities are all scalar
  - We have tacitly assumed that the grain property is uniform – the same for all grains.
- In case we use scalar quantities both ‘extreme’ cases led to the same results.
- The two assumptions are not very realistic.
  - Neither quantities are scalar, nor they are usually uniform.
  - Tensorial quantities more appropriate.
  - They might differ from one grain to another.
- What we’ll do next:
  - We use tensorial quantities in mechanics (stress, strain, modulus ...)
  - We’ll re-examine the two extreme cases using tensorial quantities.

Not scalars but tensors.

Stress is represented by more general notation called "2nd rank tensor", and the same is applied to strain, elastic compliance & modulus.

*To retain the simplicity on our analyses, I'd suggest to use "matrix notations" for these tensors.

* Also, let's reduce the dimensionality. Say, instead of using 3 x 3 matrix for stress, let's use [1x2] columnal matrix. Also, for strain. For elastic compliance & modulus, lets use [2 x 2] matrix.

* This is similar to that we use 2D plane material rather than 3D volumic material. (Not exactly the same)

Now, the elasticity constitutive law becomes…

$\sigma = C^{el} \cdot \varepsilon^{el}$

or

$\varepsilon^{el} = M^{el} \sigma$

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \end{bmatrix} = \begin{bmatrix} C^{el}_{11} & C^{el}_{12} \\ C^{el}_{21} & C^{el}_{22} \end{bmatrix} \begin{bmatrix} \varepsilon^{el}_1 \\ \varepsilon^{el}_2 \end{bmatrix}$$

$$\boxed{\sigma_i = C^{el}_{ij} \varepsilon^{el}_j}$$

Einstein's summation convention

The same applies to aggregate,

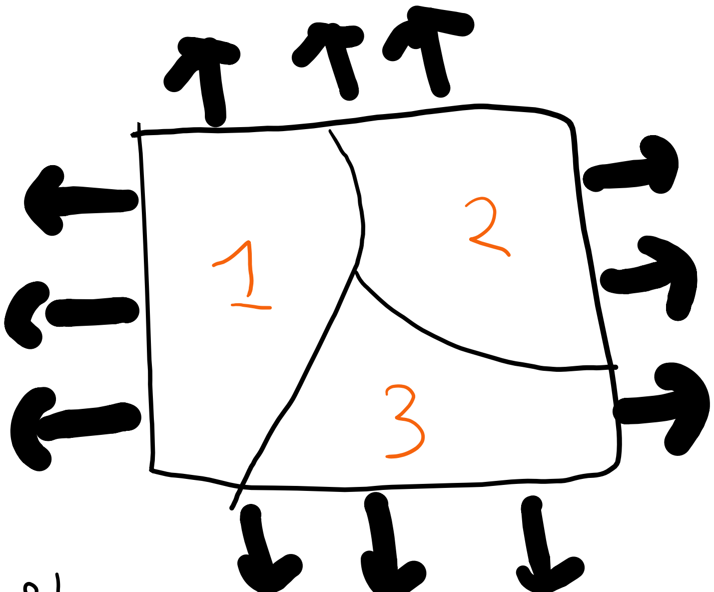
$\bar{\sigma} = \bar{C}^{el} \cdot \bar{\varepsilon}^{el}$

$$\begin{bmatrix} \bar{\sigma}_1 \\ \bar{\sigma}_2 \end{bmatrix} = \begin{bmatrix} \bar{C}^{el}_{11} & \bar{C}^{el}_{12} \\ \bar{C}^{el}_{21} & \bar{C}^{el}_{22} \end{bmatrix} \begin{bmatrix} \bar{\varepsilon}^{el}_1 \\ \bar{\varepsilon}^{el}_2 \end{bmatrix}$$

$$\bar{\sigma}_i = \bar{C}^{el}_{ij} \bar{\varepsilon}^{el}_j$$

Einstein's summation convention.

Let's apply the constitutive equations in the matrix notation



$f^1 = \frac{1}{3}$

$f^2 = \frac{1}{3}$

$f^3 = \frac{1}{3}$

*Each member has the same weights.

Q.

$\bar{\sigma}_1 = 10\,\mathrm{MPa}$ | $\bar{\varepsilon}_1^{el}$?

$\bar{\sigma}_2 = 15\,\mathrm{MPa}$ | $\bar{\varepsilon}_2^{el}$?

$C_{ij}^{el} = \begin{bmatrix} 200 & 0 \\ 0 & 100 \end{bmatrix}$

$M_{ij}^{el} = (C_{ij}^{el})^{-1} = \begin{bmatrix} \frac{1}{200} & 0 \\ 0 & \frac{1}{100} \end{bmatrix}$

$C_{12}^{el} = C_{21}^{el} = 0$, $C_{11}^{el} = 200$, $C_{22}^{el} = 100$ [GPa]

The 1st extreme case & The 2nd extreme case | $\bar{C}^{el} = \langle C^{el} \rangle$ & $\bar{M}^{el} = \langle M^{el} \rangle$

Case 3-1. $\bar{C}^{el} = \langle C^{el} \rangle$

$$\rightarrow \bar{C}^{el}_{ij} = \langle C^{el}_{ij} \rangle = \sum_{gr=1}^{gr=3} C^{el,gr}_{ij} \times w^{gr}$$

weight

$$\begin{bmatrix} \bar{C}^{el}_{11} & \bar{C}^{el}_{12} \\ \bar{C}^{el}_{21} & \bar{C}^{el}_{22} \end{bmatrix} = \begin{bmatrix} 200 & 0 \\ 0 & 100 \end{bmatrix} \frac{1}{3} + \begin{bmatrix} 200 & 0 \\ 0 & 100 \end{bmatrix} \frac{1}{3} + \begin{bmatrix} 200 & 0 \\ 0 & 100 \end{bmatrix} \frac{1}{3}$$

$$= \begin{bmatrix} 200 & 0 \\ 0 & 100 \end{bmatrix} \quad \text{unit: [GPa]}$$

$$\bar{M}^{el}_{ij} = (\bar{C}^{el})^{-1} \rightarrow \frac{1}{200 \times 100 - 0 \times 0} \begin{bmatrix} 100 & 0 \\ 0 & 200 \end{bmatrix}$$

$$\rightarrow \bar{M}^{el}_{ij} = \frac{1}{20000} \begin{bmatrix} 100 & 0 \\ 0 & 200 \end{bmatrix} = \begin{bmatrix} \frac{1}{200} & \\ & \frac{1}{100} \end{bmatrix}$$

Case 3-1. $\tilde{C}^{el} = \langle C^{el} \rangle$

$$\rightarrow \bar{C}^{el}_{ij} = \langle C^{el}_{ij} \rangle = \sum_{gr=1}^{gr=3} C^{el,gr}_{ij} \times w^{gr}$$

weight

$$\begin{bmatrix} \bar{C}^{el}_{11} & \bar{C}^{el}_{12} \\ \bar{C}^{el}_{21} & \bar{C}^{el}_{22} \end{bmatrix} = \begin{bmatrix} 200 & 0 \\ 0 & 100 \end{bmatrix} \frac{1}{3} + \begin{bmatrix} 200 & 0 \\ 0 & 100 \end{bmatrix} \frac{1}{3} + \begin{bmatrix} 200 & 0 \\ 0 & 100 \end{bmatrix} \frac{1}{3}$$

$$= \begin{bmatrix} 200 & 0 \\ 0 & 100 \end{bmatrix}$$

unit : [GPa]

$$\bar{M}^{el}_{ij} = \begin{bmatrix} \frac{1}{200} & 0 \\ 0 & \frac{1}{100} \end{bmatrix} [GPa]^{-1}$$

//

$$\bar{\varepsilon}^{el}_{i} = \bar{M}^{el}_{ij} \, \bar{\sigma}_j$$

$$\bar{\varepsilon}^{el}_{i} = \begin{bmatrix} \frac{1}{200} & 0 \\ 0 & \frac{1}{100} \end{bmatrix} \begin{bmatrix} 10 \\ 15 \end{bmatrix} = \begin{bmatrix} \frac{10}{200,000} \\ \frac{15}{100,000} \end{bmatrix} = \begin{bmatrix} \frac{1}{20} 10^{-3} \\ \frac{3}{20} 10^{-3} \end{bmatrix}$$

$[GPa]^{-1}$ [MPa]

Case 3-2. $\tilde{M}^{el} = \langle M^{el} \rangle$

$$\to \bar{M}^{el}_{ij} = \langle M^{el}_{ij} \rangle = \sum_{gr=1}^{gr=3} M^{el,gr}_{ij} \times w^{gr}$$

weight

$$\begin{bmatrix} \bar{M}^{el}_{11} & \bar{M}^{el}_{12} \\ \bar{M}^{el}_{21} & \bar{M}^{el}_{22} \end{bmatrix} = \begin{bmatrix} 1/200 & 0 \\ 0 & 1/100 \end{bmatrix} \frac{1}{3} + \begin{bmatrix} 1/200 & 0 \\ 0 & 1/100 \end{bmatrix} \frac{1}{3} + \begin{bmatrix} 1/200 & 0 \\ 0 & 1/100 \end{bmatrix} \frac{1}{3}$$

$$= \begin{bmatrix} 1/200 & 0 \\ 0 & 1/100 \end{bmatrix}$$

unit : [GPa]

The same resultant $\tilde{M}^{el}_{ij} = \begin{bmatrix} 1/200 & 0 \\ 0 & 1/100 \end{bmatrix}$.

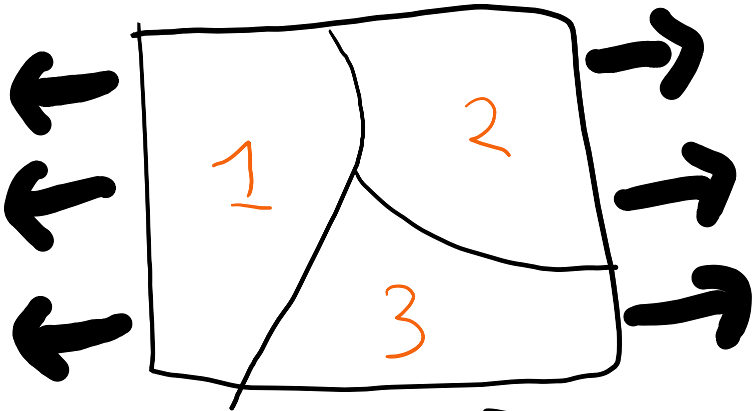
There, even for "multidimensional" problem with multidimensional σ, ε^{el}, M^{el} and C^{el}, the extreme cases 1 & 2 lead to the same result.

Summary

- Both scalar quantities and tensorial quantities led to the same conclusions:
  - The two extreme cases 1 and 2 led to the same result.
- This almost suggests that the weighted average estimation of polycrystal property is reasonable
  - We'll study further on this issue later and will show that this is **not always true**.
- Think about the assumption we made:
  - The local properties are 'uniform' – thus not changing from one grain to another.
  - This is a very *special* treatment.
  - Generally in polycrystal, from a grain to another, grains exhibit different properties – (anisotropy and different orientation).
  - We'll study this more general situation on the two extreme cases.

Something we can do is check if the non-uniform case would also lead to the same result for the two extreme cases.

Case 3-3.



loaded $\bar{\sigma} = 10\,\mathrm{MPa}$

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what is $\bar{\varepsilon}^{el}$?

~~각 grain의 moduli: $\mathbb{C}^{el} = 200\ [GPa]$ 로 주어졌다~~.

$C^{el,1} = 200 \quad C^{el,2} = 150, \; C^{el,3} = 250$

각 grain의 성질 $\mathbb{C}^{el}$ 은 주어졌지만, 전체 다결정의 성질 $\bar{\mathbb{C}}^{el}$은 주어지지 않았다. 다결정의 $\bar{\varepsilon}^{el} = \bar{\mathbb{M}}^{el}\bar{\sigma}$ 구성방정식을 통해 탄성 변형량을 알기 위해서는 다결정의 성질 (compliance of polycrystal) $\bar{\mathbb{M}}^{el}$ 을 알아야 한다.

If we apply the 1st extreme cases

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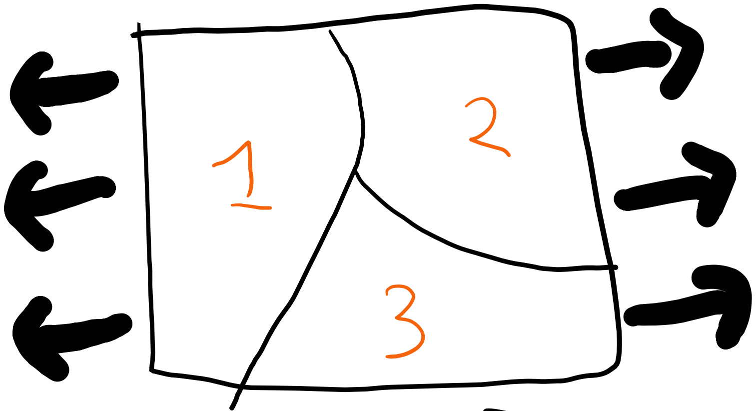
$$= 200\ [GPa]$$

$$\bar{M}^{el} = (\bar{C}^{el})^{-1} = \frac{1}{200}\ [GPa^{-1}]$$; Elastic compliance

$$\bar{\varepsilon}^{el} = \bar{M}^{el} \cdot \bar{\sigma} \longrightarrow \bar{\varepsilon}^{el} = \frac{1}{200}\frac{1}{[GPa]} \times 10 [MPa] = 5.0 \times 10^{-3}$$

Case 3-4.



loaded $\bar{\sigma} = 10\ MPa$

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$\rightarrow M^{el,1} = 1/200 \quad M^{el,2} = 1/150 \quad M^{el,3} = 1/250$

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$0.0052\cdots\ [GPa^{-1}]$

Elastic compliance

$$\bar{\varepsilon}^{el} = \bar{M}^{el} \cdot \bar{\sigma} \longrightarrow \bar{\varepsilon}^{el} = 0.0052 \frac{1}{[GPa]} \times 10\,[MPa] = 5.22 \times 10^{-3}$$

If grain's property is not uniform, the two extreme cases lead to "Different" results.

If we think about a polycrystal steel, we know what elastic moduli it has from the literature.

Fully annealed polycrystal steel, naturally has the same crystal elastic moduli. Then, why bother?