FACULTÉ DES SCIENCES ET TECHNOLOGIES
Département Physique

Université de Lille

Imperfections – deformation and microstructures in polycrystals

Sébastien Merkel
Professor, Physics Department
UMET Laboratory (Unité Matériaux et Transformations)
sebastien.merkel@univ-lille.fr

4- Polycrystals properties

Objectives

How to evaluate average properties of a polycrystal ?

- Elasticity 101
- Other tensorial properties
- Elasticity in random polycrystals
  - Mean calculations
  - Reuss/Voigt/Hill averages
  - Other models
- Elasticity in textured polycrystals
  - Calculation
  - Examples and applications.

4- Polycrystals properties
a- Elasticity 101

Stress and strain tensors

Tensor :

- can be thought of as a generalization of a vector
- used to represent quantities for which component change with transformation of space

Stress tensor: rank-2 tensor to describe stress applied to a material.

Strain tensor: rank-2 tensor to describe tensor applied to a material.

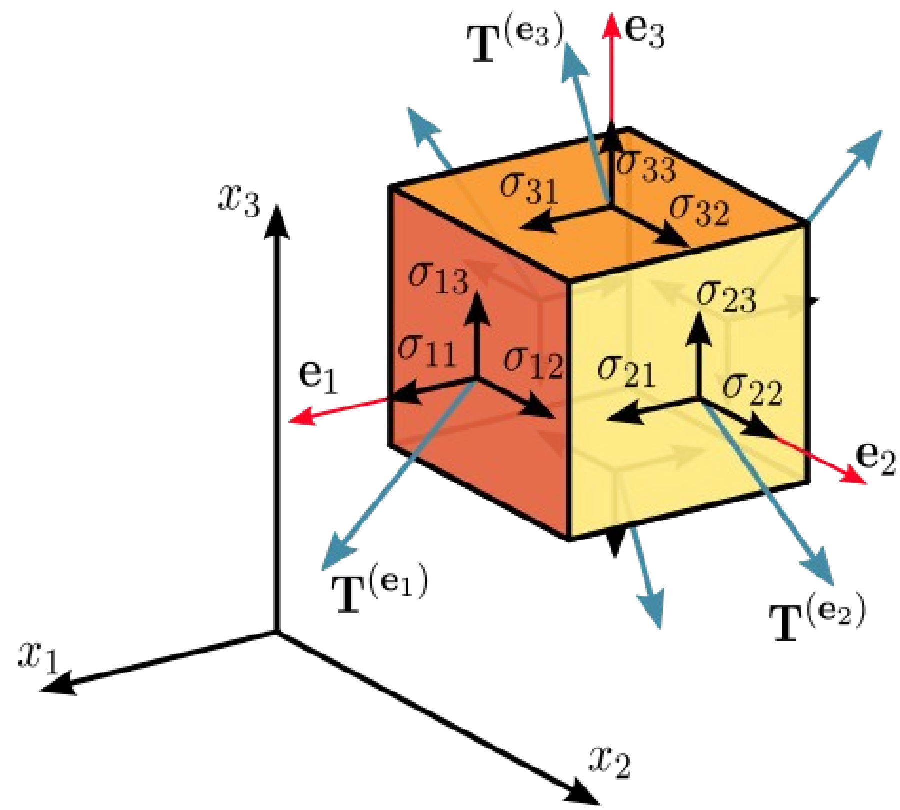


Illustration wikipedia

Tensor rotation

Rank-0 tensor:

- Quantity that is independent of the reference frame
- Examples : pressure, temperature, etc.

Rank-1 tensor:

- 3 quantities that transform like a regular vector
- Mathematically: $T'_i = a_{ik} T_k$
- Example: position vector

Rang-2 tensor:

- Mathematically: $T'_{ij} = a_{ik} a_{jl} T_{kl}$ (attention: it is not a simple matrix multiplication)
- Matrix notation: $T' = a T {}^t a$
- Examples: stress and strain tensors

Rank-4 tensor:

- Mathematically: $T'_{ijkl} = a_{im} a_{jn} a_{ko} a_{lp} T_{mnop}$
- Example: elastic constants or compliances

Elasticity

- Linear relationship between the stress tensor $\boldsymbol{\sigma}$ and the strain tensor $\boldsymbol{\varepsilon}$
- Tensorial expression
  - $\boldsymbol{\sigma} = C:\boldsymbol{\varepsilon}$
  - $\boldsymbol{\varepsilon} = S:\boldsymbol{\sigma}$
- *C*: elastic constants - *S*: elastic compliances
- $C = S^{-1}$ (much easier to evaluate in the reduced Voigt form)
- Component expression
  - $\sigma_{ij} = C_{ijkl}\, \varepsilon_{kl}$;
  - $\varepsilon_{ij} = S_{ijkl}\, \sigma_{kl}$;
- Young’s modulus = stress in tension / strain in tension
- Anisotropic Young’s modulus : $1/S'_{1111}$, where S' is expressed in an appropriate reference frame
- Appropriate reference frame: reference frame in which tension is along axis *1*.

Questions

- What is the difference between elastic and plastic behavior
- Define the Young's modulus
- What is a tensor?
- Define what are the stress, strain, and elastic tensors.
- What is the reduced Voigt notation?
- What is the effect of crystal symmetry on the Cij's?
- Spell out the elastic tensor for a cubic, hexagonal and orthorhombic crystal systems.

Other tensors in physics (1)

Property	Symbol	Field	Response	Type#
Tensors of Rank 0 (Scalars)				
Specific Heat	C	ΔT	$T\Delta S$	E1
Tensors of Rank 1 (Vectors)				
Electrocaloric	p_i	E_i	ΔS	E3
Magnetocaloric	q_i	H_i	ΔS	E3
Pyroelectric	p'_i	ΔT	D_i	E3
Pyromagnetic	q'_i	ΔT	B_i	E3
Tensors of Rank 2				
Thermal expansion	α_{ij}	ΔT	ϵ_{ij}	E6
Piezocaloric effect	α'_{ij}	σ_{ij}	ΔS	E6
Dielectric permittivity	κ_{ij}	E_j	D_i	E6
Magnetic permeability	μ_{ij}	H_j	B_i	E6
Optical activity	g_{ij}	$l_i l_j$	G	E6
Magnetoelectric polarization	λ_{ij}	H_j	D_i	E9
Converse magnetoelectric polarization	λ'_{ij}	E_j	B_i	E9
Electrical conductivity (resistivity)	σ_{ij} (ρ_{ij})	E_j (j_j)	j_i (E_i)	T6
Thermal conductivity	K_{ij}	$\nabla_j T$	h_i	T6
Diffusivity	D_{ij}	$\nabla_j c$	m_i	T6
Thermoelectric power	Σ_{ij}	$\nabla_j T$	E_i	T9
Hall effect	R_{ij}	B_j	ρ^a_i	T9

Source: T. Rollet – Original source: M. De Graef

Other tensors in physics (2)

Tensors of Rank 3				
Piezoelectricity	d_{ijk}	σ_{jk}	D_i	E18
Converse piezoelectricity	d'_{ijk}	E_k	ϵ_{ij}	E18
Piezomagnetism	Q_{ijk}	σ_{jk}	B_i	E18
Converse piezomagnetism	Q'_{ijk}	H_k	ϵ_{ij}	E18
Electro-optic effect	r_{ijk}	E_k	$\Delta\beta_{ij}$	E18
Nernst tensor	Σ_{ijk}	$\nabla_j T B_k$	E_i	T27
Tensors of Rank 4				
Elasticity	s_{ijkl} (c_{ijkl})	σ_{kl} (ϵ_{kl})	ϵ_{ij} (σ_{ij})	E21
Electrostriction	γ_{ijkl}	$E_k E_l$	ϵ_{ij}	E36
Photoelasticity	q_{ijkl}	σ_{kl}	$\Delta\beta_{ij}$	E36
Kerr effect	p_{ijkl}	$E_k E_l$	$\Delta\beta_{ij}$	E36
Magnetoresistance	ξ_{ijkl}	$B_k B_l$	ρ^s_{ij}	T36
Piezoresistance	Π_{ijkl}	σ_{kl}	$\Delta\rho_{ij}$	T36
Magnetothermoelectric power	Σ_{ijkl}	$\nabla_j T B_k B_l$	E_i	T54
Second order Hall effect	ρ_{ijkl}	$B_j B_k B_l$	ρ^2_i	T30
Tensors of Rank 6				
Third order elasticity	c_{ijklmn}	$\epsilon_{kl}\epsilon_{mn}$	σ_{ij}	E56

Source: T. Rollet – Original source: M. De Graef

4- Polycrystals properties
b- Elasticity in random polycrystals

Average properties

Polycrystal, with an infinite number of grains, randomly oriented and covering the full orientation space

- Isotropic material
- 2 independent elastic coefficients:
  - E and ν ;
  - K and G ;
  - ...

Matrix form:

$$S = \begin{bmatrix} \frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G} \end{bmatrix}$$

$$G = \frac{E}{2(1+\nu)}$$

$$K = \frac{E}{3(1-2\nu)}$$

Average calculations

Contribution of a single crystallite

- $C'_{11} = C'_{1111} = g_{1i}g_{1j}g_{1k}g_{1l}\, C_{ijkl}$
- $C'_{11} = g_{11}g_{11}g_{11}g_{11}\, C_{1111} + g_{11}g_{11}g_{11}g_{12}\, C_{1112} + \ldots.$
- $C'_{11} = (g_{11})^4\, C_{1111} + 2(g_{11})^2(g_{12})^2\, C_{1122} + 2(g_{11})^2(g_{13})^2\, C_{1133}$
  $+ 4(g_{11})^2 g_{12}g_{13}\, C_{1123} + \ldots.$

Contribution of all crystallites

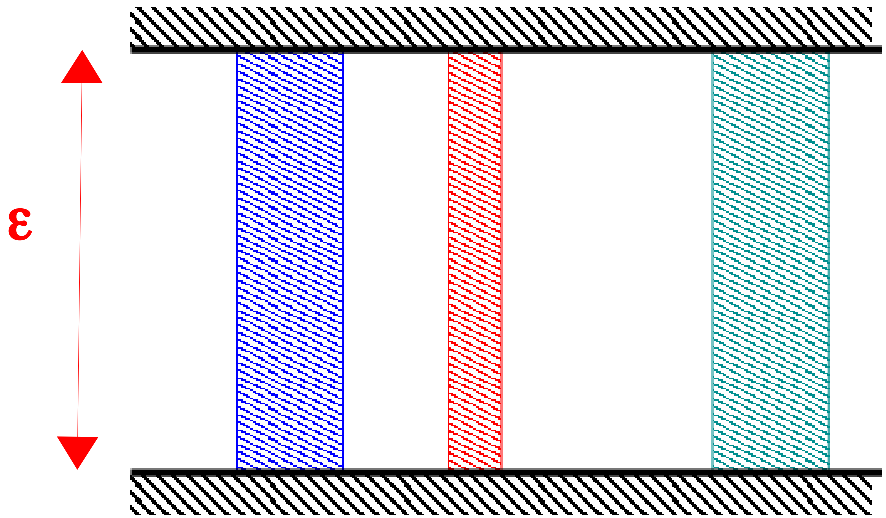
- $\langle C'_{11}\rangle = \langle (g_{11})^4\rangle\, C_{1111} + 2\langle (g_{11})^2(g_{12})^2\rangle\, C_{1122} +$
  $2\langle (g_{11})^2(g_{13})^2\rangle\, C_{1133} + 4\langle (g_{11})^2 g_{12}g_{13}\rangle C_{1123} + \ldots.$
- $\langle\rangle$: averaging over all orientations → over the full Euler space

A few results

- $\langle g_{11}\rangle = 0$; $\langle (g_{11})^2\rangle = 1/3$; $\langle (g_{11})^4\rangle = 1/5$; $\langle (g_{11})^2(g_{12})^2\rangle = 1/15$

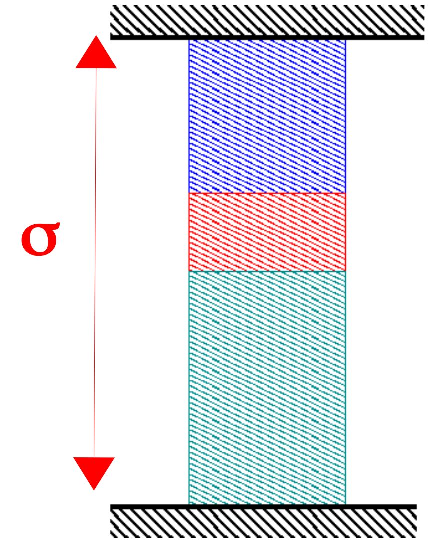
Reuss-Voigt-Hill averages

Voigt average



Deformation is equal in all grains
« iso-strain average »

Reuss average



Stress is equal in all grains
« iso-stress average »

Hill average

In 1952, Hill showed that the Reuss and Voigt means are bounds, bounds between which is the true polycrystal. He suggests using a new average, the mean of the Voigt and Reuss bounds.

Voigt mean

Voigt mean: strain tensor is the same in all crystallites.

Hooke’s law applied as σ = C:ε since the strain tensor is know.

Voigt mean → average of the C_{ij}’s

Result:

$$\langle C'_{11}\rangle = \frac{3}{15}(C_{11}+C_{22}+C_{33})+\frac{2}{15}(C_{12}+C_{13}+C_{23})+\frac{4}{15}(C_{44}+C_{55}+C_{66})$$

$$\langle C'_{12}\rangle = \frac{1}{15}(C_{11}+C_{22}+C_{33})+\frac{4}{15}(C_{12}+C_{13}+C_{23})-\frac{2}{15}(C_{44}+C_{55}+C_{66})$$

$$\langle C'_{44}\rangle = \frac{1}{15}(C_{11}+C_{22}+C_{33})-\frac{1}{15}(C_{12}+C_{13}+C_{23})+\frac{3}{15}(C_{44}+C_{55}+C_{66})$$

One can validate that $<C'_{44}> = (<C'_{11}>-<C'_{12}>)/2$ (isotropic material).
Other parameters (E, K, G, ν) can be calculated from $<C'_{11}>$, $<C'_{12}>$, and $<C'_{44}>$.

Reuss mean

Reuss mean: stress tensor is the same in all crystallites.

Hooke's law applied as ε = S:σ since the stress tensor is know.

Reuss mean → average of the S_{ij}'s

Result:

$$\langle S'_{11} \rangle = \frac{3}{15}(S_{11}+S_{22}+S_{33}) + \frac{2}{15}(S_{12}+S_{13}+S_{23}) + \frac{4}{15}(S_{44}+S_{55}+S_{66})$$

$$\langle S'_{12} \rangle = \frac{1}{15}(S_{11}+S_{22}+S_{33}) + \frac{4}{15}(S_{12}+S_{13}+S_{23}) - \frac{2}{15}(S_{44}+S_{55}+S_{66})$$

$$\langle S'_{44} \rangle = \frac{1}{15}(S_{11}+S_{22}+S_{33}) - \frac{1}{15}(S_{12}+S_{13}+S_{23}) + \frac{3}{15}(S_{44}+S_{55}+S_{66})$$

The C_{ij}'s are then calculating by inverting the S_{ij} matrix.

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Other bounds

Since the 1960's other bounds have been suggested

- Hashin & Shtrickman, 1967
- Geometric mean : Moraviec, 1989, Matthies and Humbert, 1987

Their solutions are less far apart that those of Reuss and Voigt.

As a matter of fact the Hill average is much faster to evaluate. None of them is truly better anyway.

The Reuss, Voigt, Hill, and geometric means are compatible with texture calculations. The Hashin & Shtrickman bound is not.

Example

Young and shear moduli for some metals.

Reuss and Voigt bounds.

Hill average.

Experimental values.

In GPa.

Module	Cuivre	Or	Fer α
E_R	109	69	193
E_V	144	87	229
E_H	127	78	211
E_{exp}	123	79	213
G_R	40	24	74
G_V	54	31	86
G_H	47	27	80
G_{exp}	46	28	83

4- Polycrystals properties
b- Elasticity in textured polycrystals

Elasticity in texture polycrystal

Polycrystal properties = average properties of all crystallites.

Random polycrystal: average properties of all orientations in space.

Oriented polycrystal: ODF-weighted average.

$$\langle C \rangle = \int C(g) f(g) dg$$

Voigt average

$$\langle S \rangle = \int S(g) f(g) dg$$

Reuss average

Not always straightforward

- Plain calculation: 81 C_{ijkl}
- With boxes of 5°x5°x5° in orientation space: 186 000 coefficients for the ODF.

There are optimized algorithms

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Polycrystal tensors: symmetry

Pay attention:

- Random polycrystal → isotropic
- Textured polycrystal → anisotropic
- Anisotropy depends on that of the single-crystal AND texture.

$$\begin{bmatrix} 230 & 135 & 135 & & & \\ & 230 & 135 & & & \\ & & 230 & & & \\ & & & 116 & & \\ & & & & 116 & \\ & & & & & 116 \end{bmatrix}$$

Elastic constants
α-iron single-crystal

α-iron
Random polycrystal

$C_{44} = (C_{11}-C_{12})/2$
Isotropic

$$\begin{bmatrix} 275 & 113 & 113 & & & \\ & 275 & 113 & & & \\ & & 275 & & & \\ & & & 81 & & \\ & & & & 81 & \\ & & & & & 81 \end{bmatrix}$$

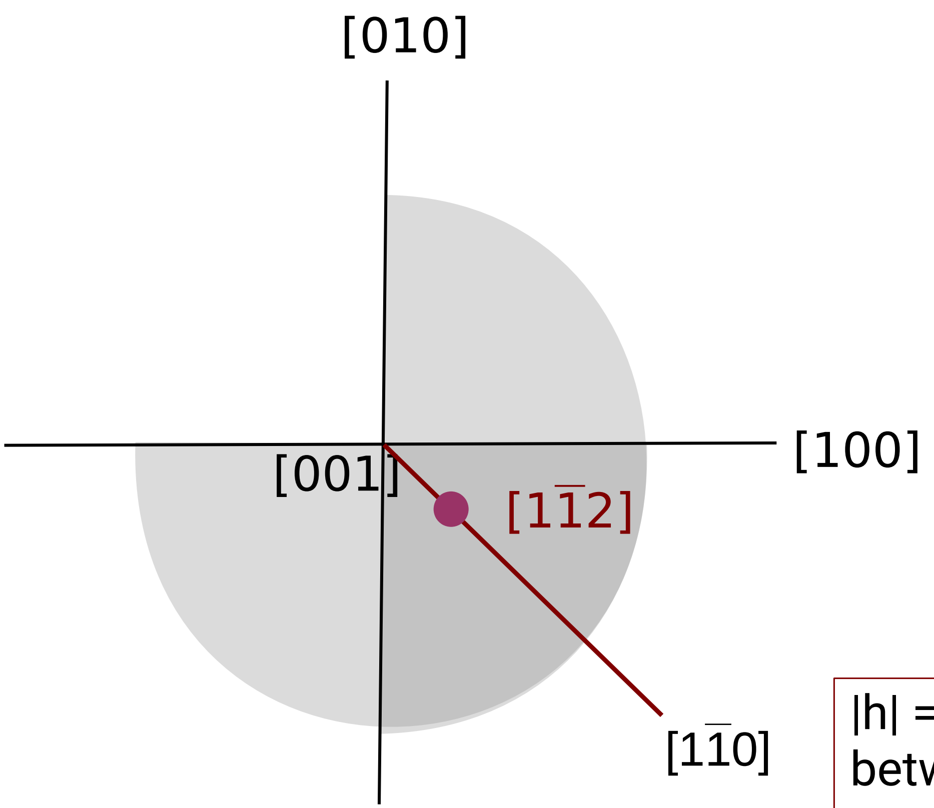
α-iron
After 100 % tensile strain

$C_{66} = (C_{11}-C_{12})/2$
Hexagonal

$$\begin{bmatrix} 279 & 114 & 107 & & & \\ & 279 & 107 & & & \\ & & 285 & & & \\ & & & 76 & & \\ & & & & 76 & \\ & & & & & 82 \end{bmatrix}$$

Interlude : back to stereograms

Practice: place the $[1\bar{1}2]$ direction on a cubic crystal stereogram



$[1\bar{1}2]\cdot[100] > 0$: $[1\bar{1}2]$ is la less that 90° from [100]

$[1\bar{1}2]\cdot[010] < 0$: $[1\bar{1}2]$ is at more than 90° from [010]

$[1\bar{1}2]\cdot[001] > 0$: $[1\bar{1}2]$ is a less than 90° of [001] (it is in the upper hemisphere)

|h| = |k| : $[1\bar{1}2]$ is in the line between [001] and $[1\bar{1}0]$

|l| > |k| : $[1\bar{1}2]$ closer to [001] than $[1\bar{1}0]$

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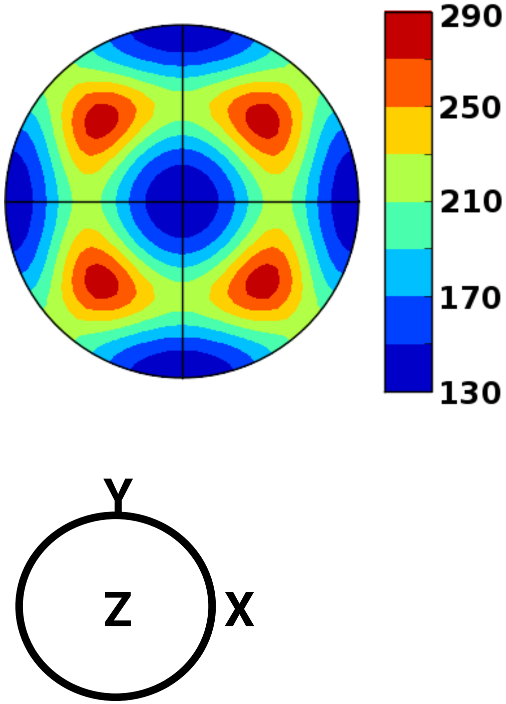
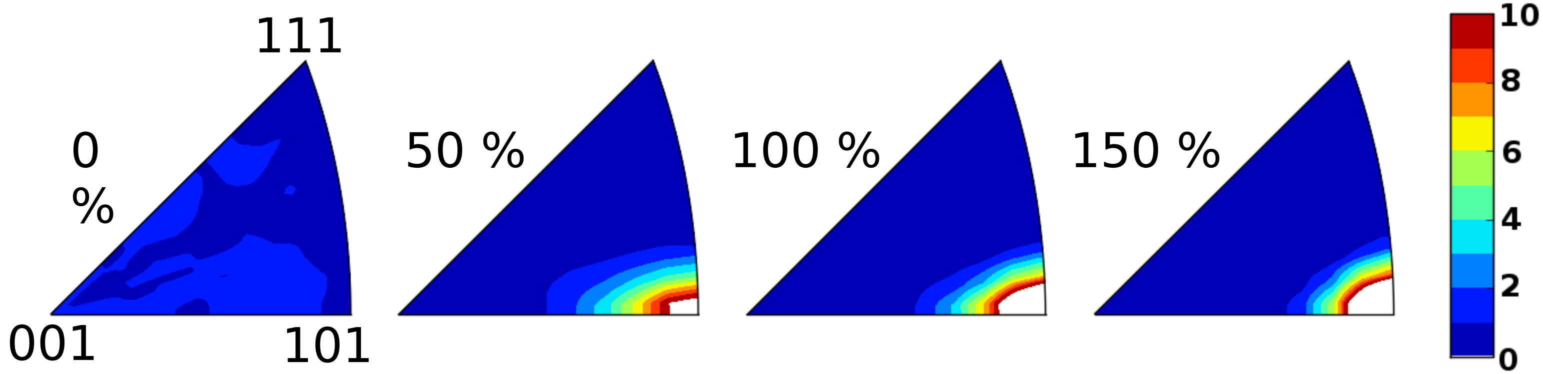
Illustration: α-iron, tensile deformation

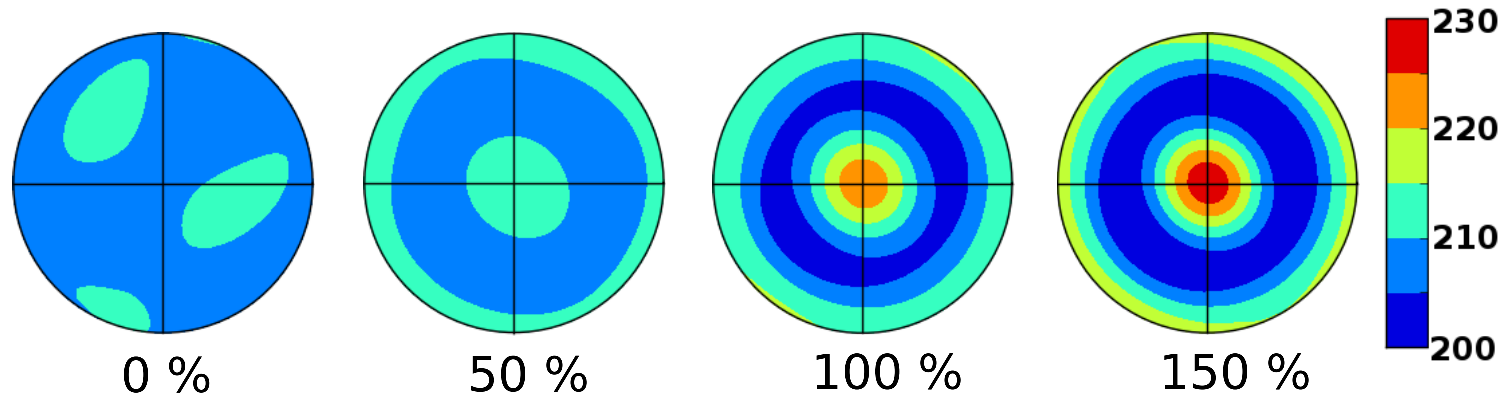
α-iron
Single-crystal
Young's
modulus
(GPa)



IPF of the tensile direction



Young's modulus (Hill)



VPSC simulation – 5000 grains

What’s been taught until now

1- Grain orientation

- Reference frames
- Euler angles, matrix representation, pole figures

2- Polycrystal orientations

- Diffraction and EBSD measurements
- Orientation distribution function
- Pole figures and inverse pole figures

3- Polycrystal properties

- Elasticity in a random polycrystal: Reuss-Voigt-Hill averages
- Elasticity in a textured polycrystal: ODF-weighted averages

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