



AKADEMIA GÓRNICZO-HUTNICZA  
IM. STANISŁAWA STASZICA W KRAKOWIE  
AGH UNIVERSITY OF SCIENCE  
AND TECHNOLOGY

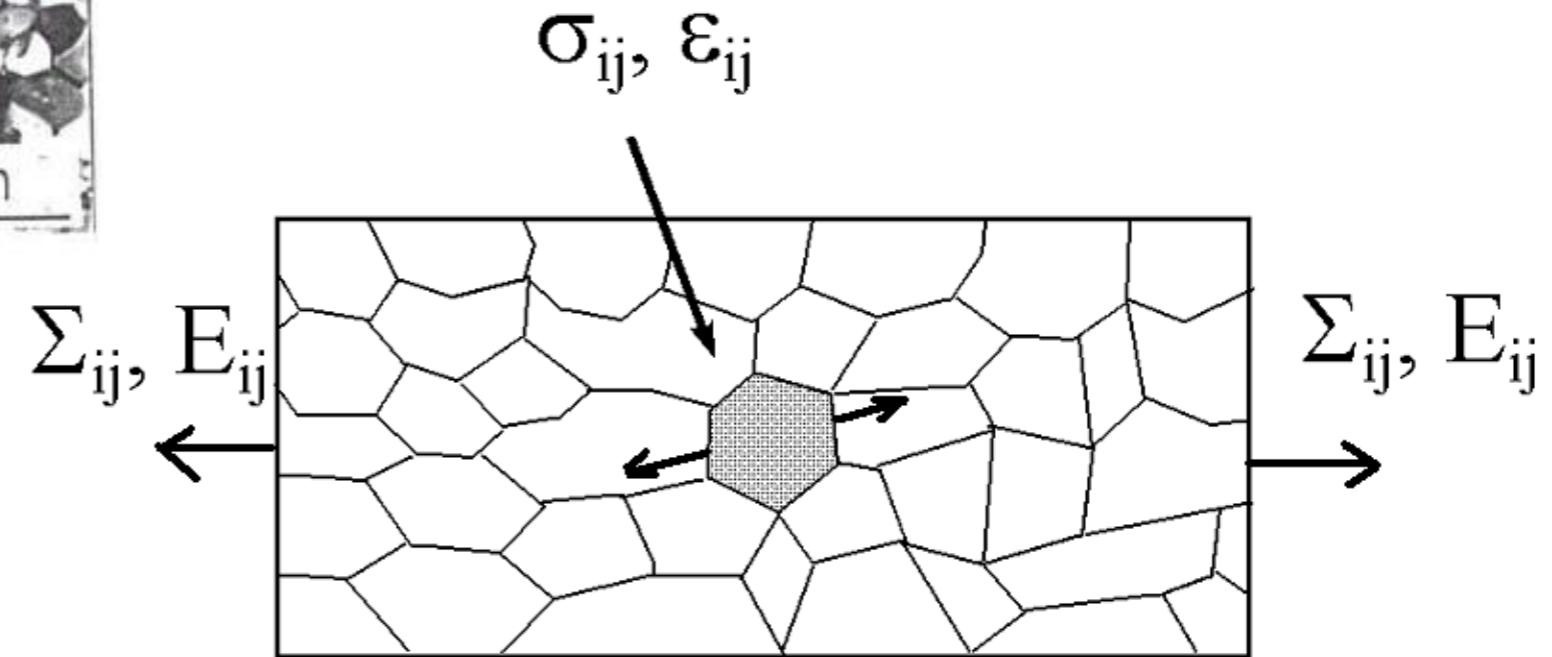
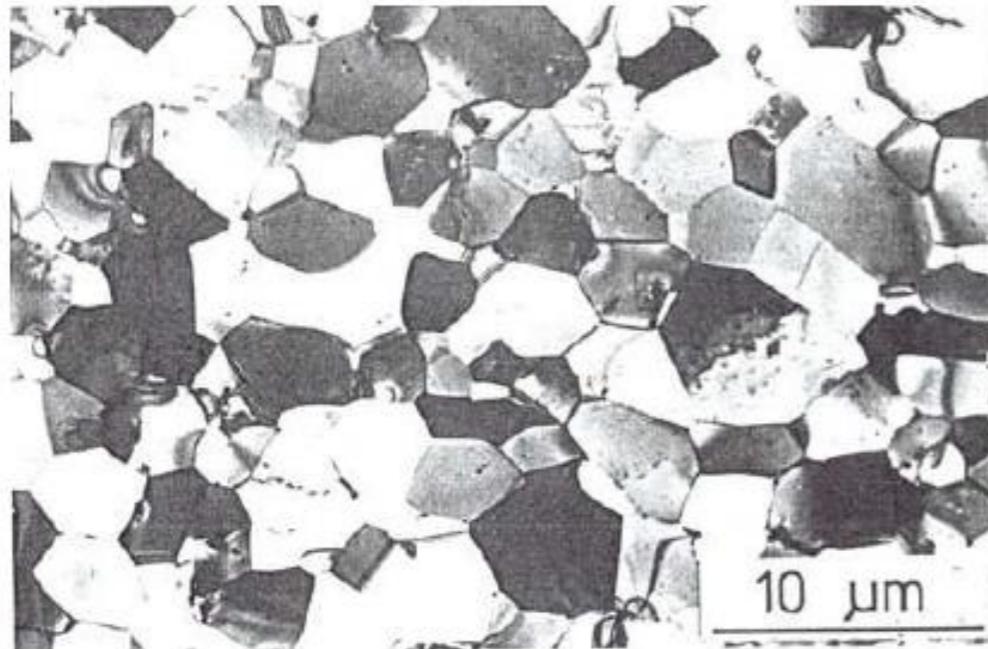
# Pomiar odkształceń sieci krystalicznej w materiałach dwufazowych poddanych obciążeniu zewnętrznemu

A. Baczmański<sup>1</sup>, A. Ludwik<sup>1</sup>, S. Wroński<sup>1</sup>, K. Wierzbanowski<sup>1</sup>, P. Kot<sup>2</sup>, M. Wroński<sup>1</sup>

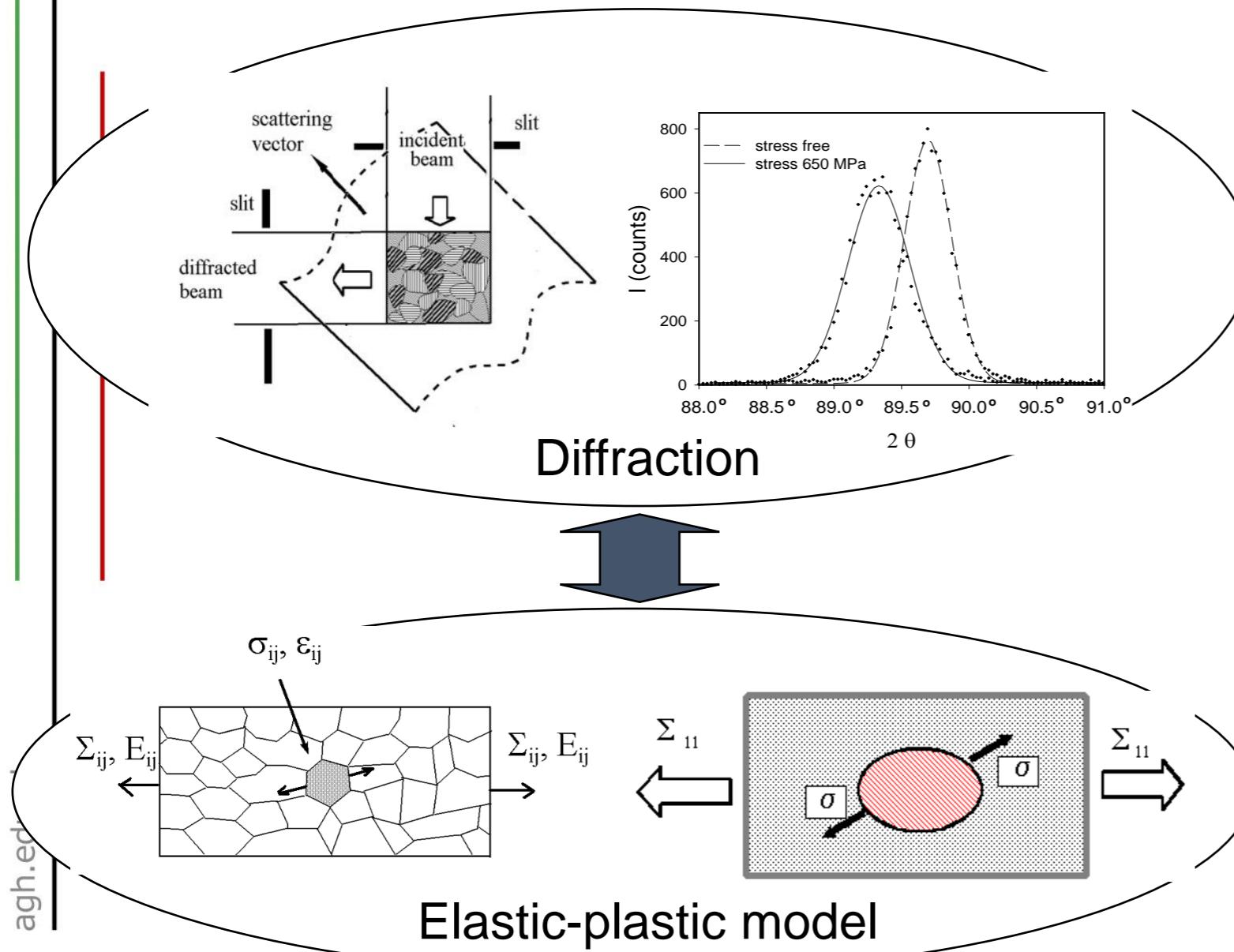
<sup>1</sup>*Akademia Górnictwo Hutnicza im. Stanisława Staszica, Wydział Fizyki i Informatyki Stosowanej,  
al. Mickiewicza 30, 30-059 Kraków, Polska,*

<sup>2</sup>*NOMATEN Centrum Doskonałości, Narodowe Centrum Badań Jądrowych, ul. A. Sołtana 7,  
05-400 Otwock-Świerk, Polska*

# Mechanical properties of polycrystalline material at grain scale



# Mechanical properties of polycrystalline material at grain scale



Lattice strains:

$$\langle \varepsilon \rangle_{hkl} = \frac{\langle d \rangle_{hkl} - d_{hkl}^0}{d_{hkl}^0}$$

$$n\lambda = 2 \langle d \rangle_{\{hkl\}} \sin \theta$$

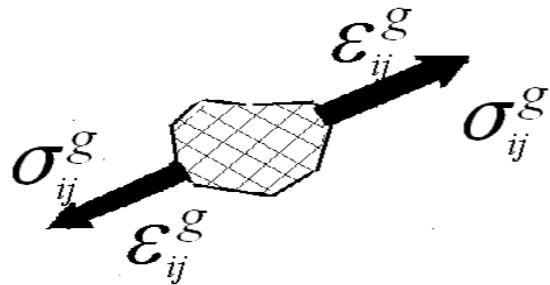
Scale transition model:

- $\dot{\varepsilon}_{ij}^g = A_{ijkl}^g \dot{E}_{kl}$

- $\dot{\sigma}_{ij}^g = B_{ijkl}^g \dot{\Sigma}_{kl}$

# Self-consistent model

## Grain scale:

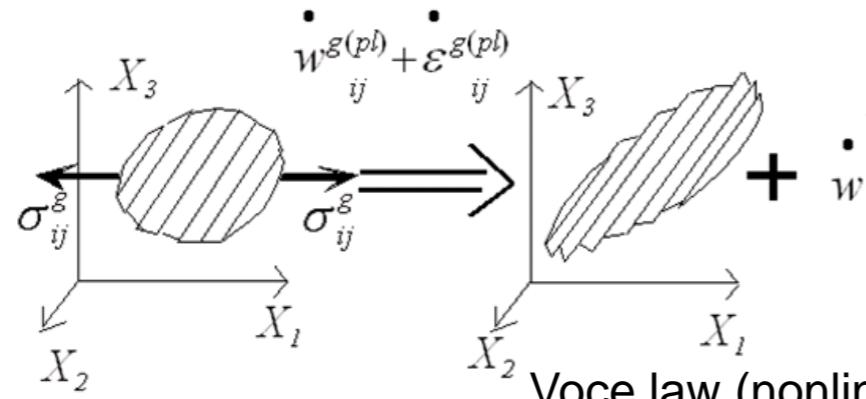


elastic deformation:  $\varepsilon_{ij}^{g(el)}$

$$\sigma_{ij}^g = c_{ijkl}^g \varepsilon_{kl}^{g(el)}$$

elastic-plastic deformation:

$$\varepsilon_{ij}^g = \varepsilon_{ij}^{g(el)} + \varepsilon_{ij}^{g(pl)}$$

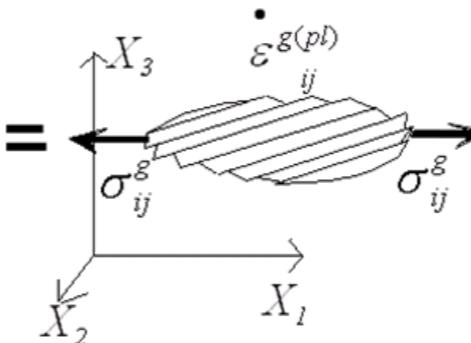


Voce law (nonlinear):

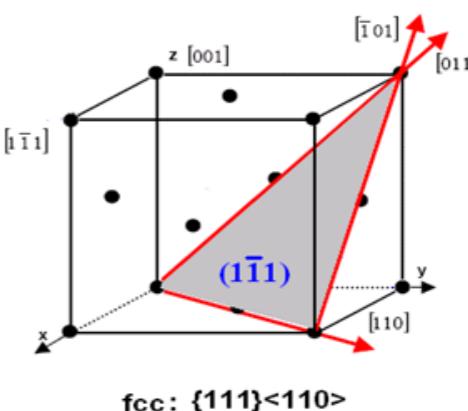
$$\tau_c^{gr} = \tau_0 + (\tau_1 + \theta_1 \xi^{gr}) \left[ 1 - \exp \left( - \frac{\theta_0}{\tau_1} \xi^{gr} \right) \right]$$

lattice rotation :

$$w_{ij}^{g(cr)}$$



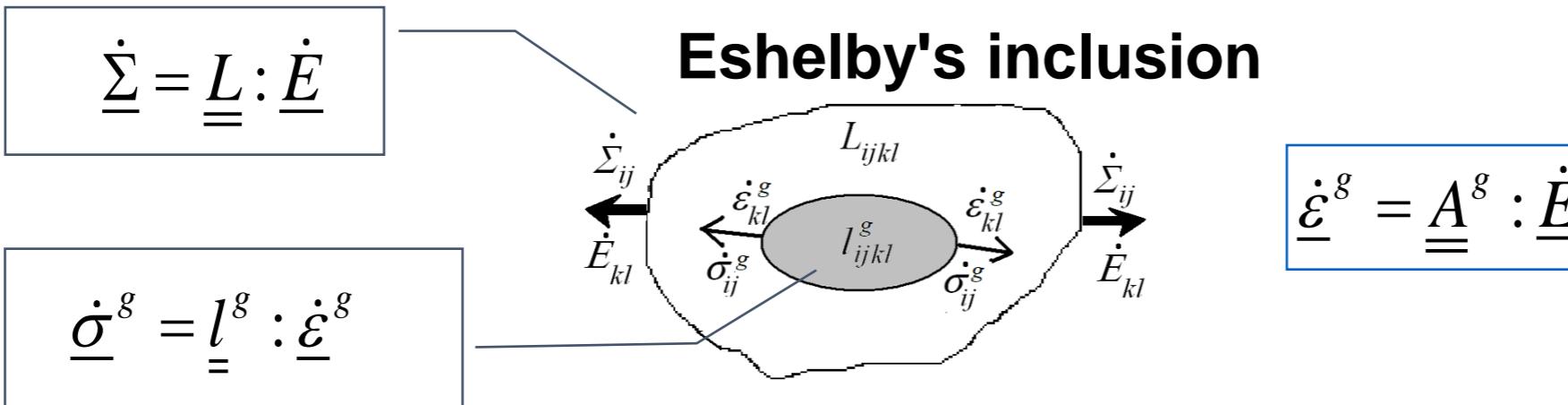
$$\sigma_{[uvw](hkl)} = \tau_c$$



# Self-consistent model

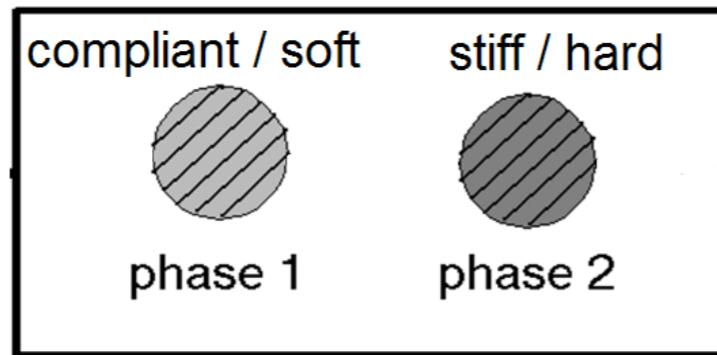
## Scale transition:

\* Homogenisation and localisation (self-consistent, Taylor....):

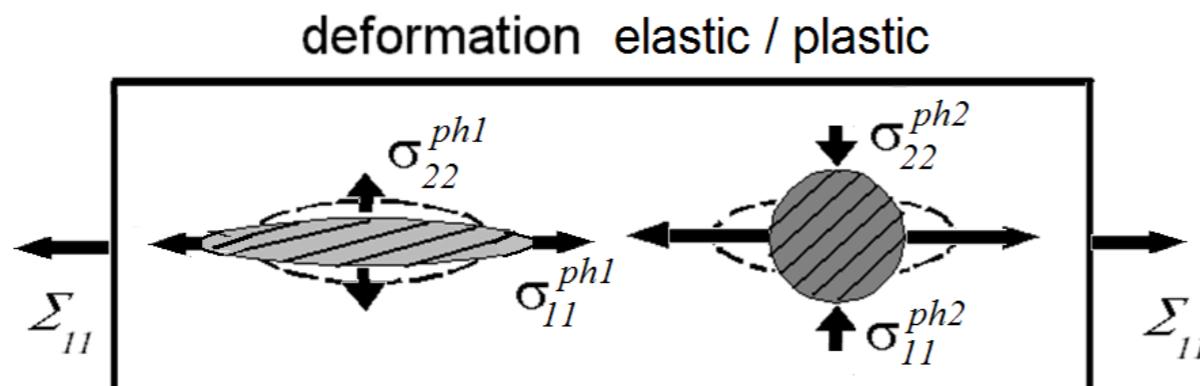


# Self-consistent model

## Stress/strain localisation: (Eshelby type model)



two phases



$$\dot{\varepsilon}_{ij}^g = A_{ijkl}^g \dot{E}_{kl} \quad \dot{\sigma}_{ij}^g = B_{ijkl}^g \dot{\Sigma}_{kl}$$

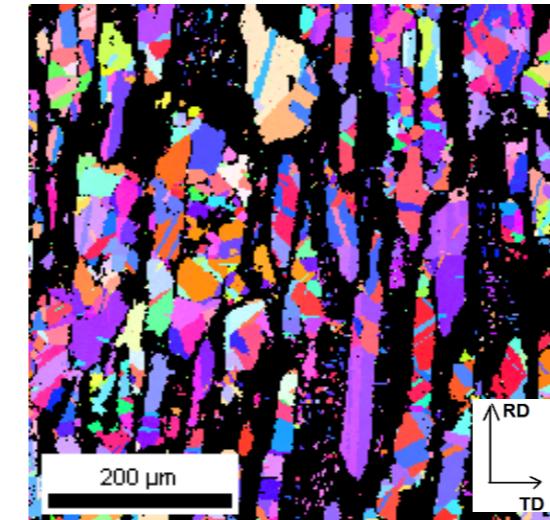
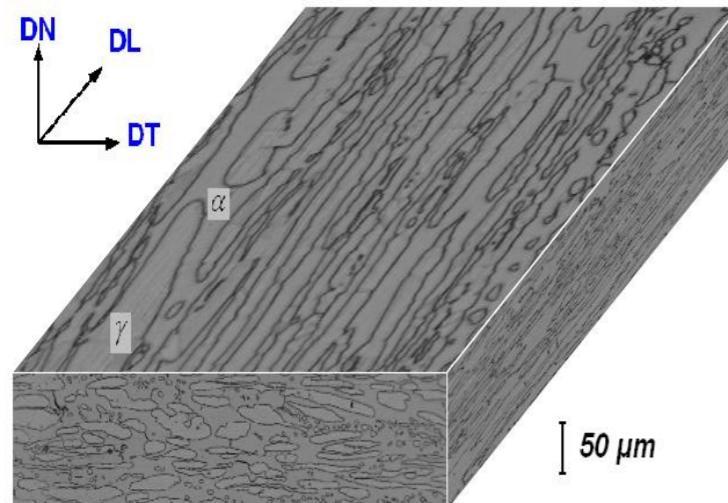
Lipinski, P. & Berveiller, M. (1989). *Int. J. Plast.*  
5, 149–172.



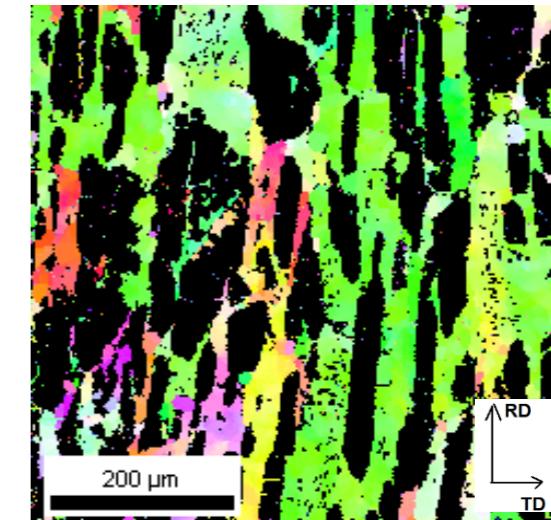
# Time of Flight in-situ tests

# Material: stainless duplex steel (aged)

50% austenite ( $\gamma$ ) and 50% ferrite ( $\alpha$ )

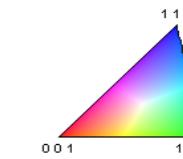


austenite



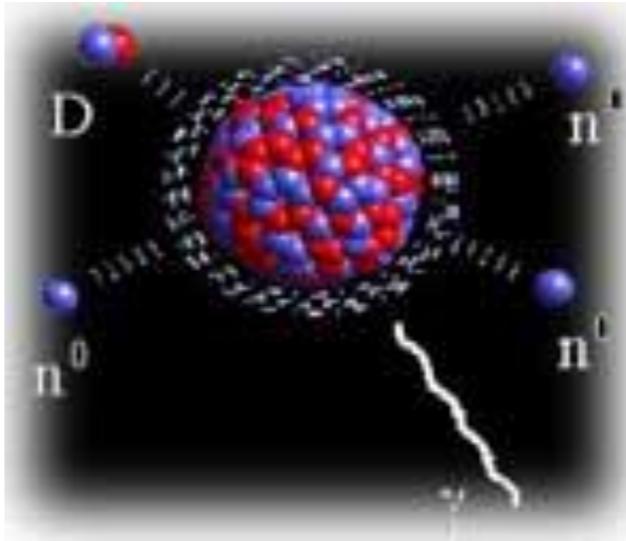
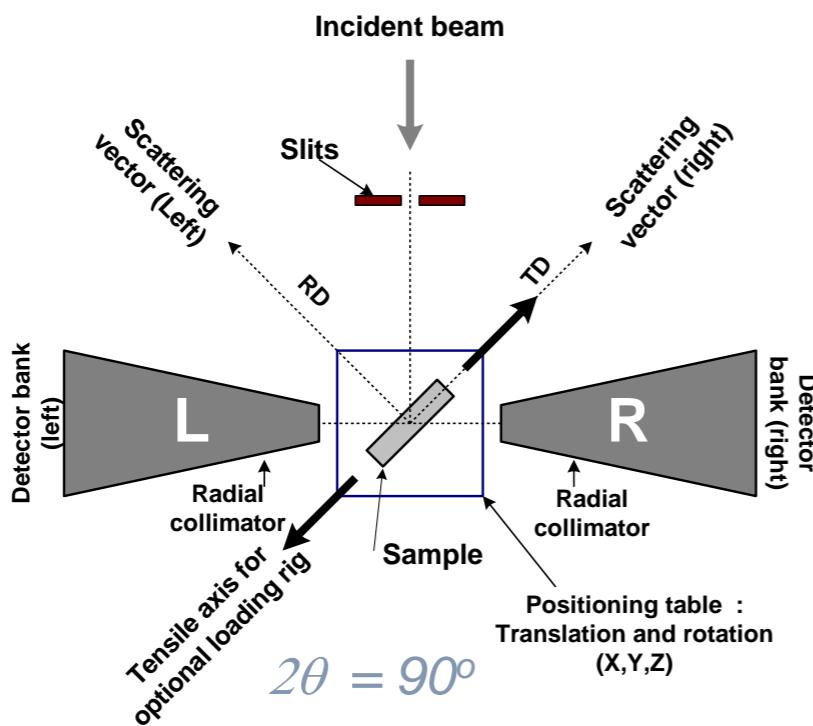
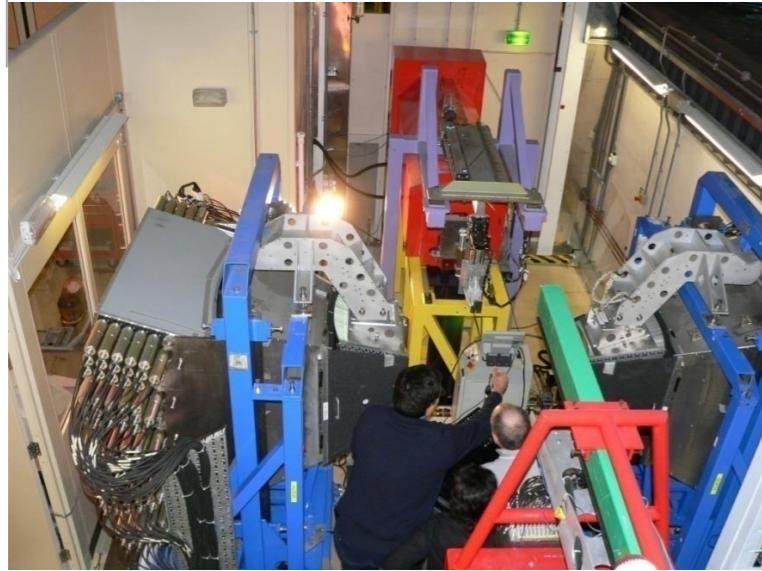
ferrite

EBSD



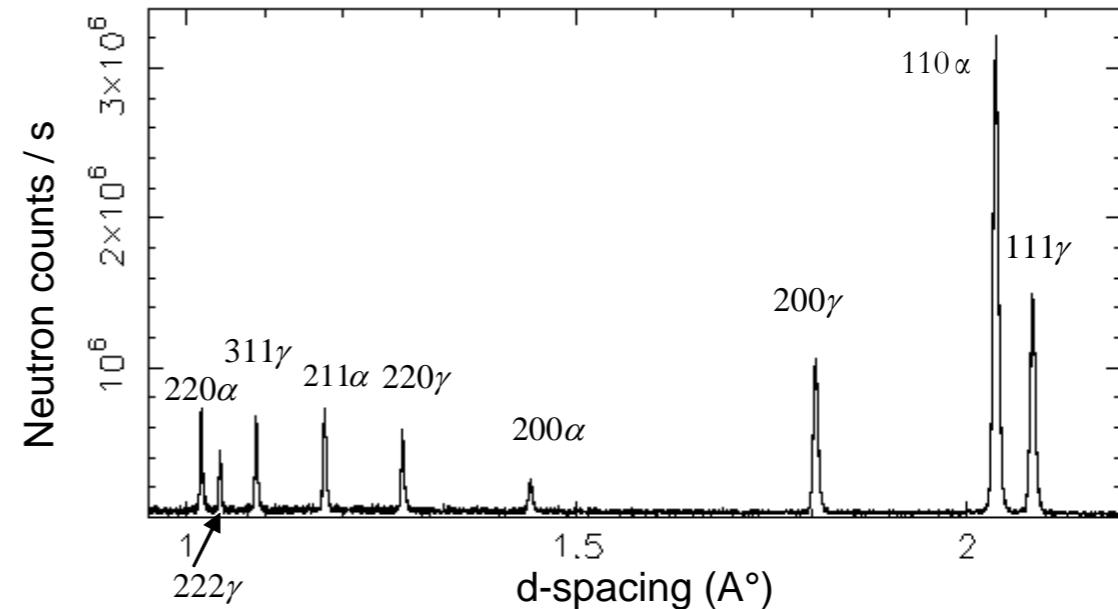
Euronorm	C	Mn	Cr	Ni	Mo	Cu	S	N
X2 Cr Ni Mo 22.5.3	0,015	1,6	22,4	5,4	2,9	0,12	0,001	<b>0,17</b>

# Duplex steel - ISIS, Rutherford Appleton Lab., UK



Spallation  
source  
TOF  
(time of flight)

$$d_{hkl} = \frac{ht}{2 \sin \theta m_n L}$$



# Duplex steel - ISIS, Rutherford Appleton Lab., UK

## Spallation source TOF (time of flight)

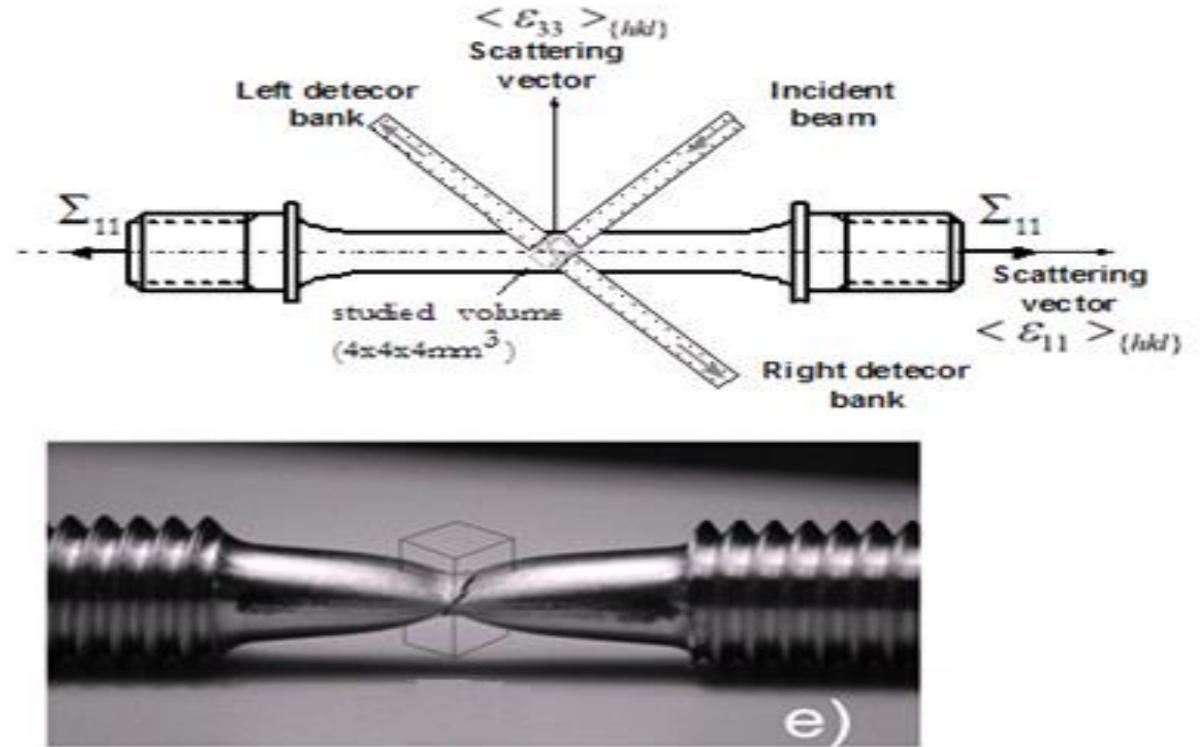
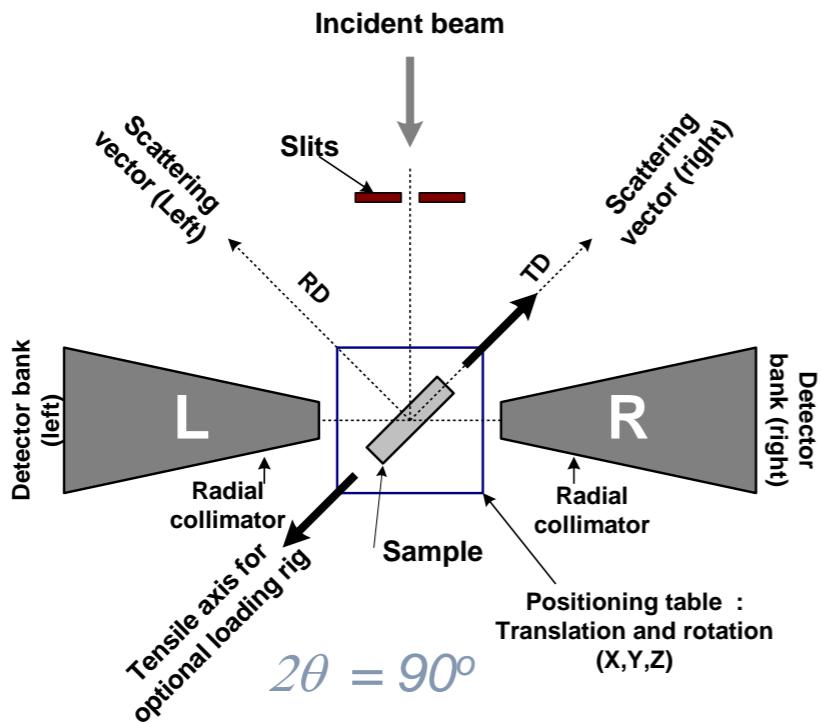
-,,in situ” tensile test

$$n\lambda = 2d_{hkl} \sin \theta$$

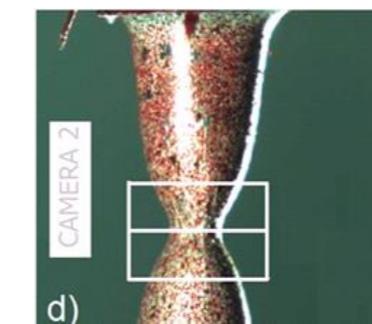
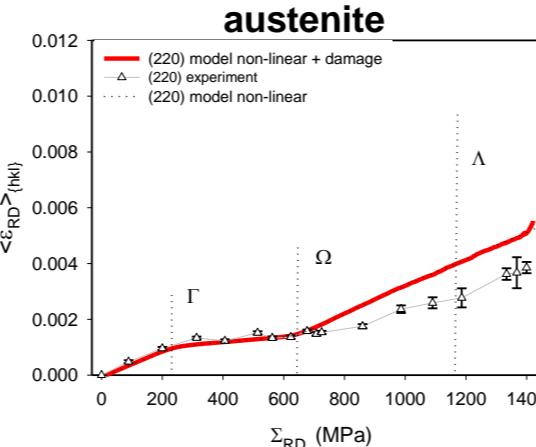
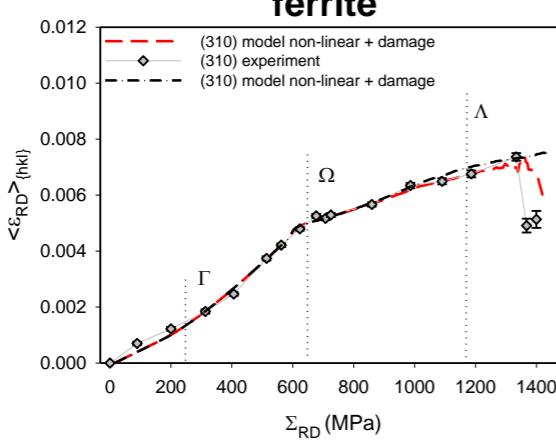
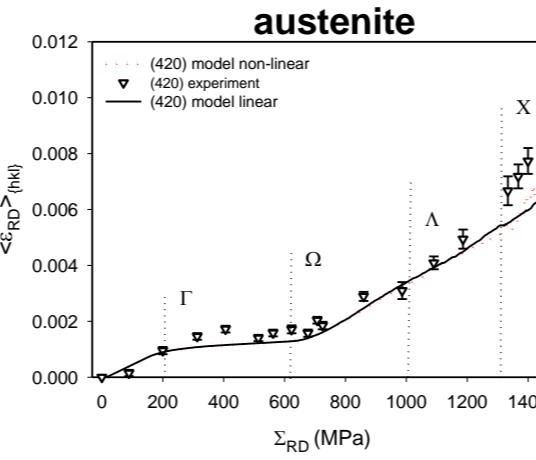
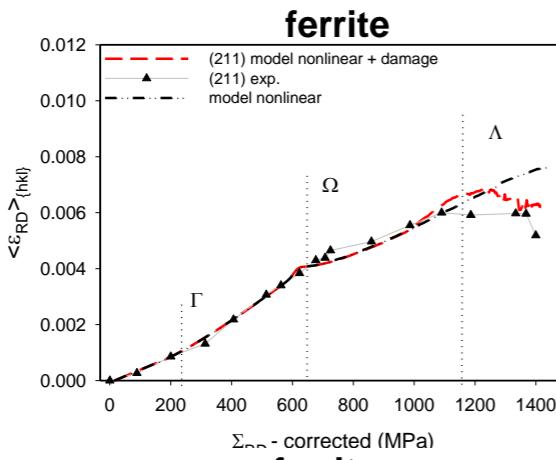
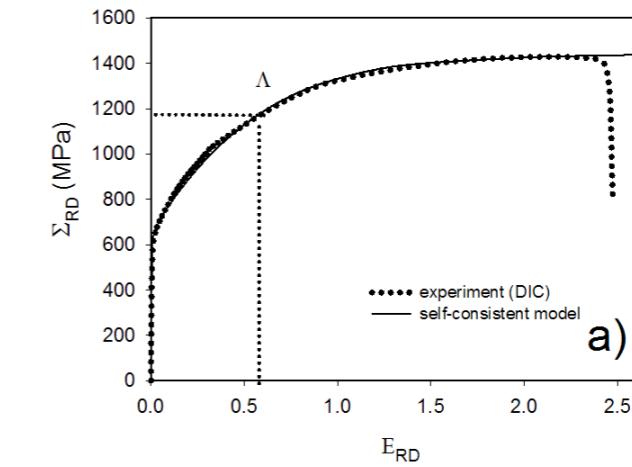
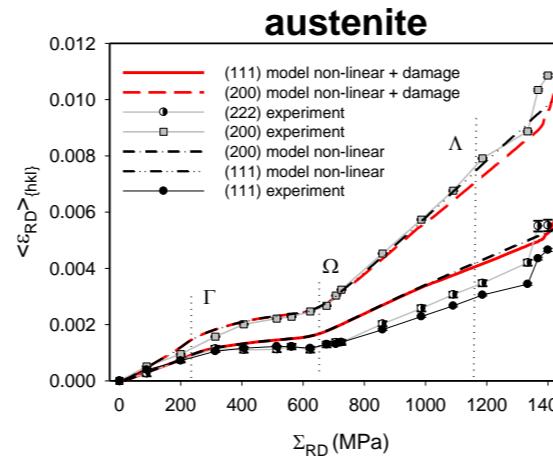
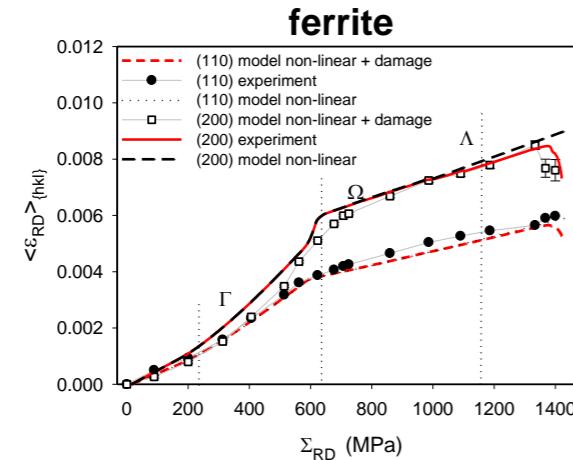
$$\lambda = \frac{h}{m_n v} = \frac{ht}{m_n L}$$

Lattice strains:

$$\langle \varepsilon \rangle_{hkl} = \frac{\langle d \rangle_{hkl} - d_{hkl}^0}{d_{hkl}^0}$$



# DUPLEX STEEL – ISIS results



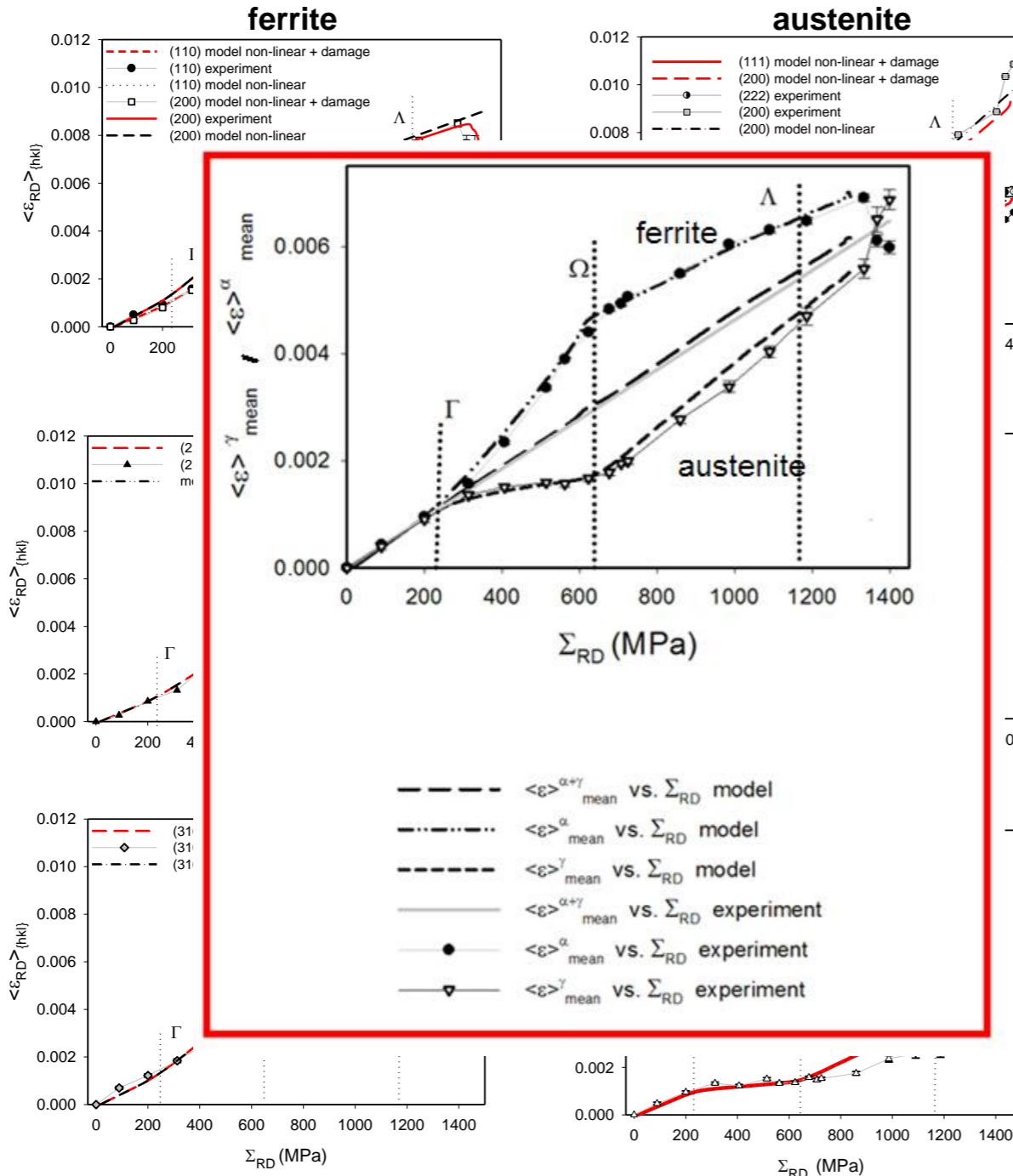
**DIC**  
Digital Image Corelation

$$\langle \varepsilon \rangle_{hkl} = \frac{\langle d \rangle_{hkl} - d_{hkl}^0}{d_{hkl}^0}$$

$d_{hkl}^0$  before loading

$\langle d \rangle_{hkl}$  under applied load

# DUPLEX STEEL – mechanical behaviour of phases



**Voce law:**

$$\tau^{gr} = \tau_0^\alpha + (\tau_1^\alpha + \theta_1^\alpha \xi^{gr}) \left[ 1 - \exp \left( - \frac{\theta_0^\alpha}{\tau_1^\alpha} \xi^{gr} \right) \right]$$

$$\tau^{gr} = \tau_0^\gamma + (\tau_1^\gamma + \theta_1^\gamma \xi^{gr}) \left[ 1 - \exp \left( - \frac{\theta_0^\gamma}{\tau_1^\gamma} \xi^{gr} \right) \right]$$

The parameters of plastic deformation (MPa)

Material	UR45N (quenched)	UR45N (aged)
$\tau_0^{(\text{ph})}$ (MPa)	Austenite	140
	Ferrite	220
$\theta_0^{(\text{ph})}$ (MPa)	Austenite	225
	Ferrite	110
$\tau_1^{(\text{ph})}$ (MPa)	Austenite	Not adjusted
	Ferrite	140
$\theta_1^{(\text{ph})}$ (MPa)	Austenite	0.3
	Ferrite	0.1

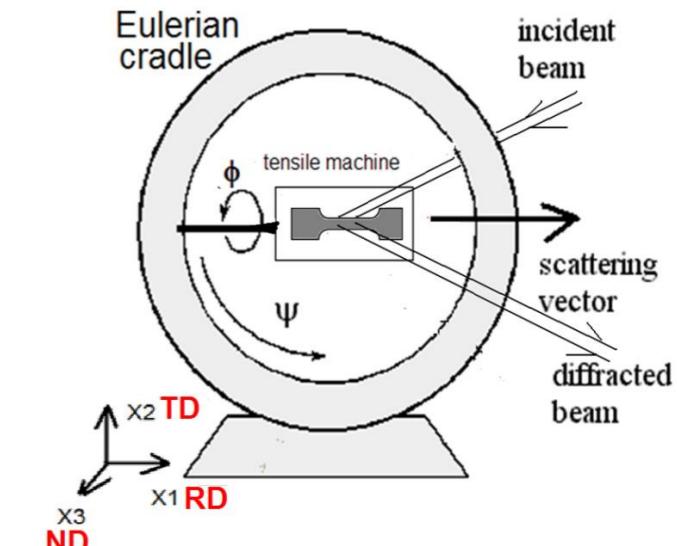
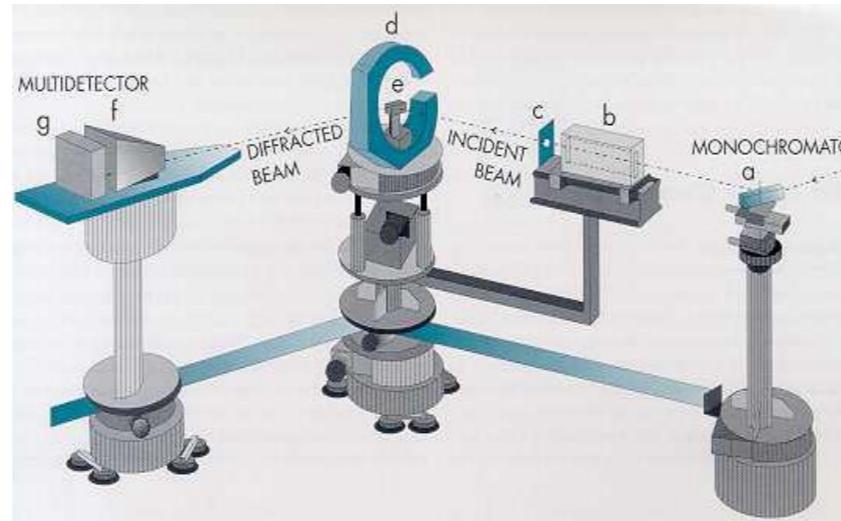
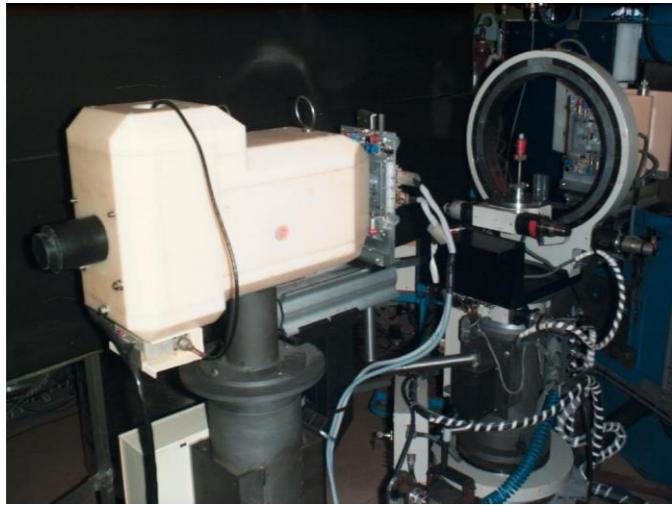


**Crystallite Group Method (*in situ*):**

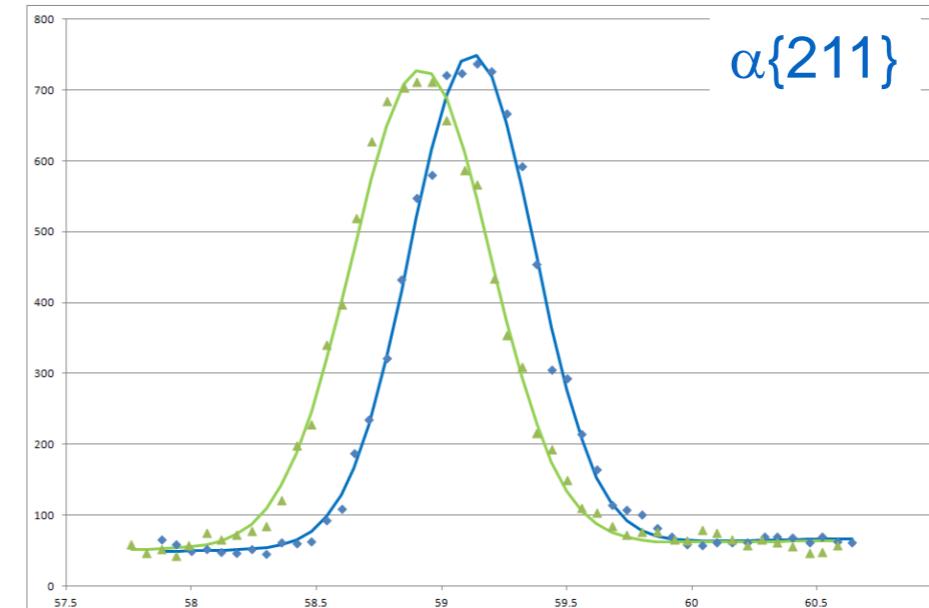
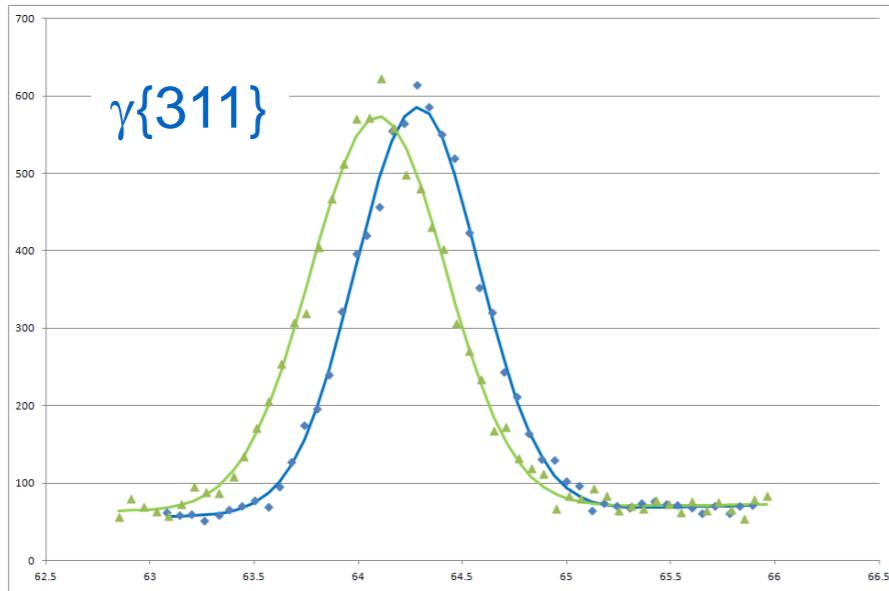
- Angular dispersion + Eulerian cradle**
- ToF**

# DUPLEX STEEL – in situ tensile test

(LLB, Saclay, 6T1, neutrons -  $2\theta$  dispersion,  $\lambda = 1.159 \text{ \AA}$ )



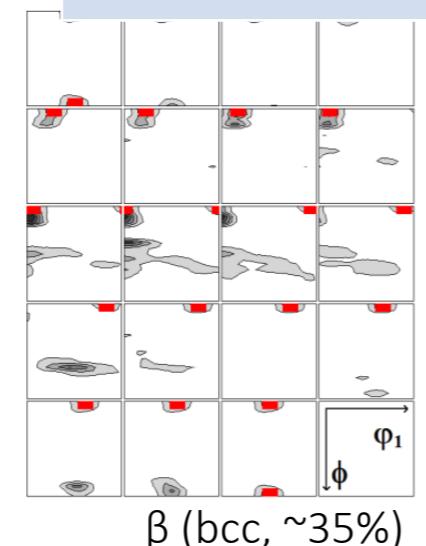
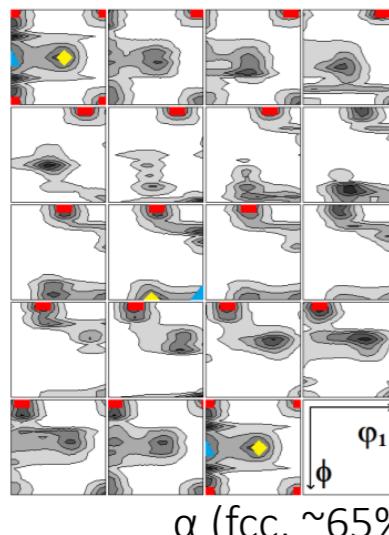
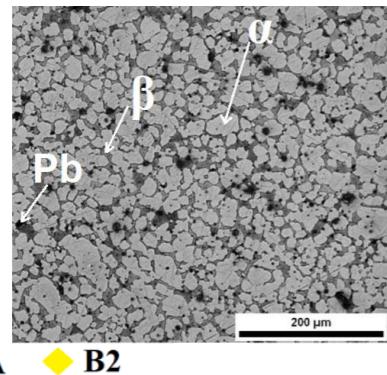
$$n\lambda = 2d_{hkl} \sin \theta$$



# Studied materials

## Two-phase brass alloy (CuZn39Pb3):

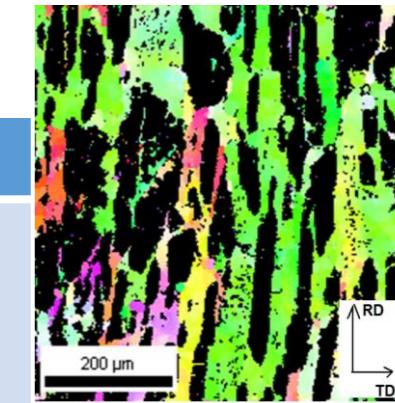
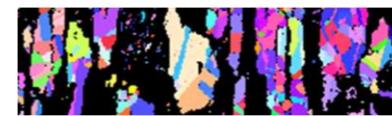
Cu	Pb	Ni	Fe	Sn	Al	Zn	other
57-59	2,5-3,5	0,30	0,50	0,30	0,005	balance	0,2 [%]
[%]	[%]	[%]	[%]	[%]	[%]		



Brass  
Hot rolled,  
annealed

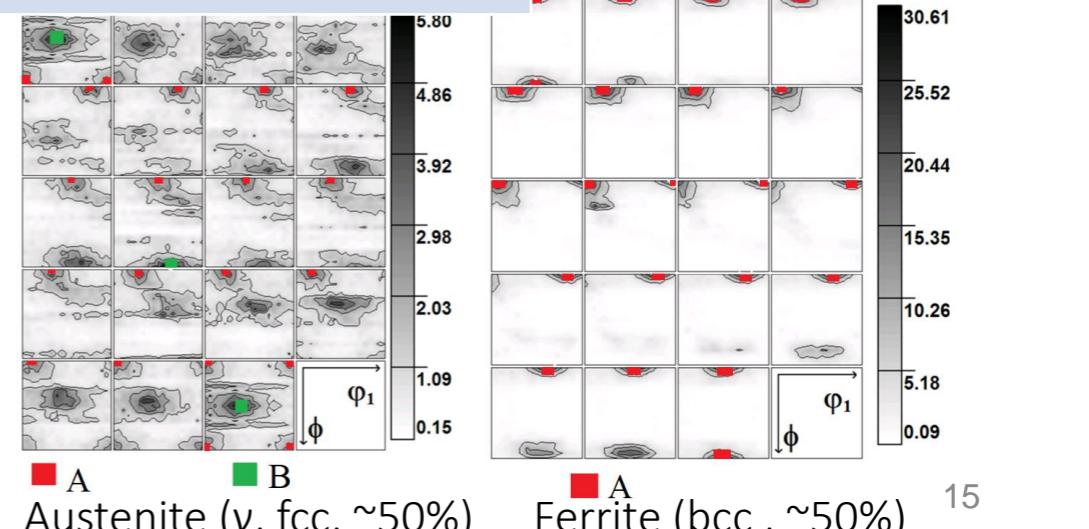
## Austeno-ferritic duplex stainless steel (UR45N):

Cr	Ni	Mo	Mn	N	Cu	C	S	Fe
22,4	5,4	2,9	1,6	0,17	0,12	0,015	0,001	balance
[%]	[%]	[%]	[%]	[%]	[%]	[%]	[%]	



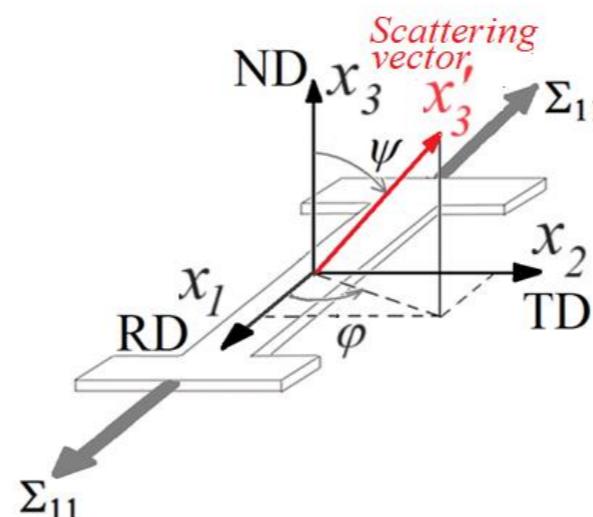
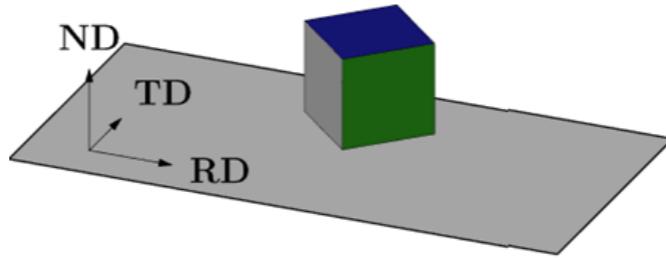
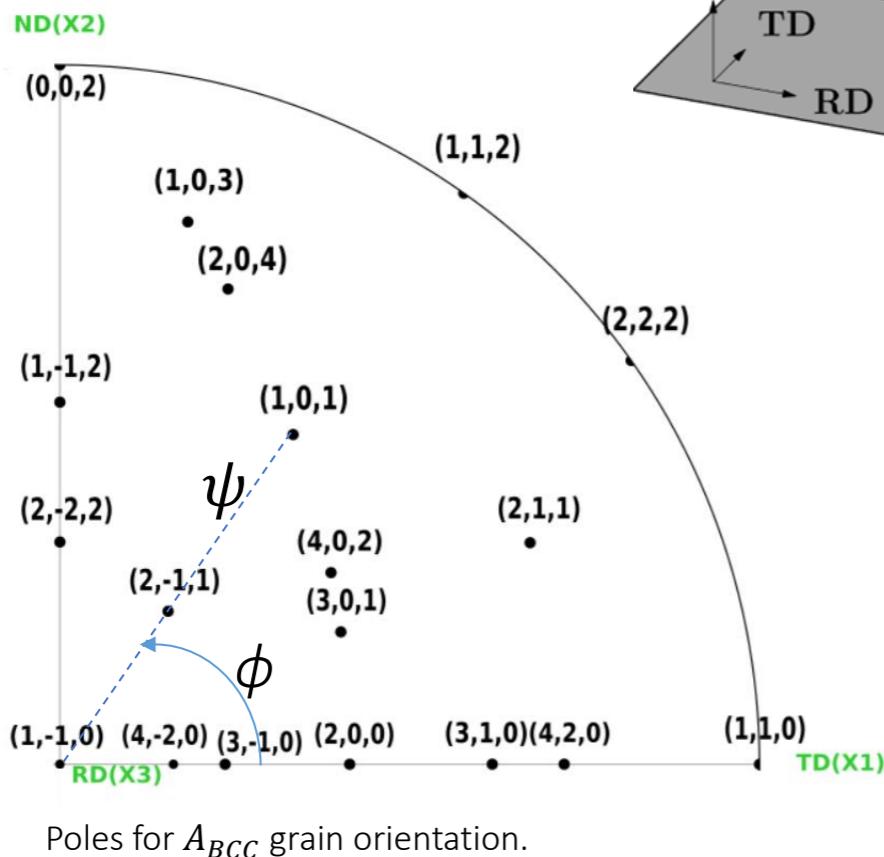
## Duplex steel

continuous casting,  
hot rolling,  
heat treated at 1050°C,  
annealed at 400°C



# Crystalite Group Method

Analysis of a group of grains with similar orientations - such groups can be determined using the poles  $P(\psi, \phi)_{\{hkl\}}$  in the pole figure.



$$\langle \varepsilon(\psi, \phi) \rangle_{\{hkl\}} = \frac{d_{\{hkl\}}^{\Sigma} - d_{\{hkl\}}^{\Sigma=0}}{d_{\{hkl\}}^{\Sigma=0}}$$

$$\langle \varepsilon(\psi, \phi) \rangle_{\{hkl\}} = a_{3k} a_{3l} s_{klji} \sigma_{ij}^{CR}$$

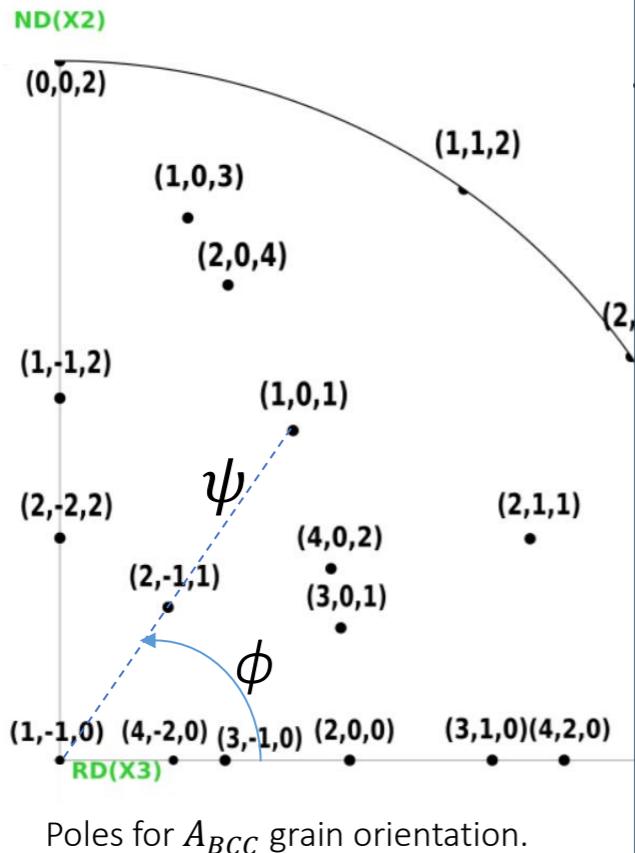
where:

$\langle \varepsilon(\psi, \phi) \rangle_{\{hkl\}}$  – lattice strain for  $P(\psi, \phi)_{\{hkl\}}$  pole,  
 $\sigma_{ij}^{CR}$  – stress tensor for the grain group,  
 $s_{klji}$  – crystallite elastic constants,  
 $a_{3k}, a_{3l}$  – components of the transformation matrix.

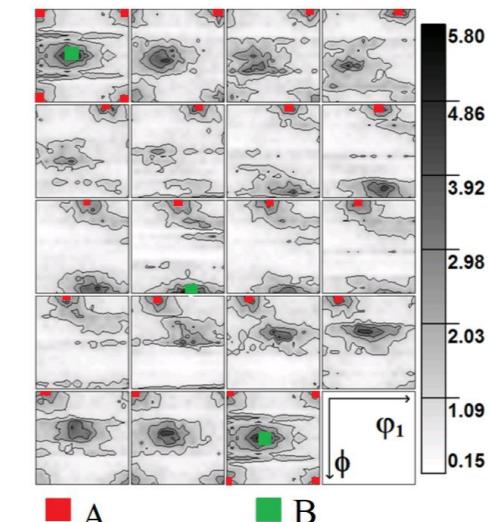
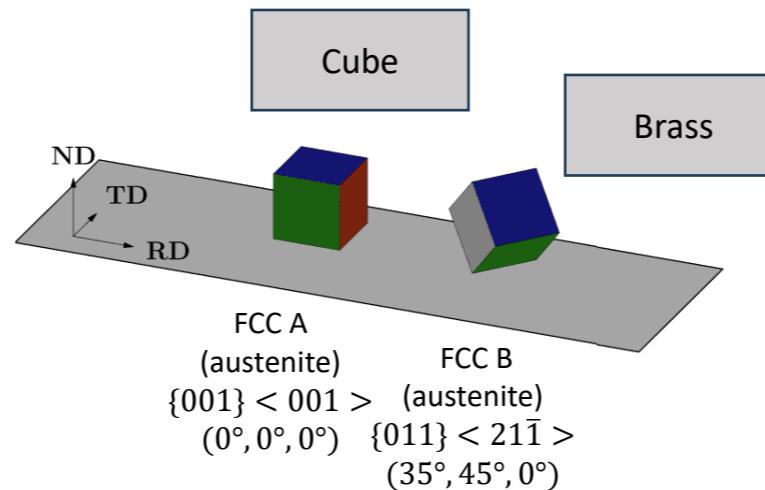
# Crystalite Group Method

$$\langle \varepsilon(\psi, \phi) \rangle_{\{hkl\}} = a_{3k} a_{3l} s_{klij} \sigma_{ij}^{CR}$$

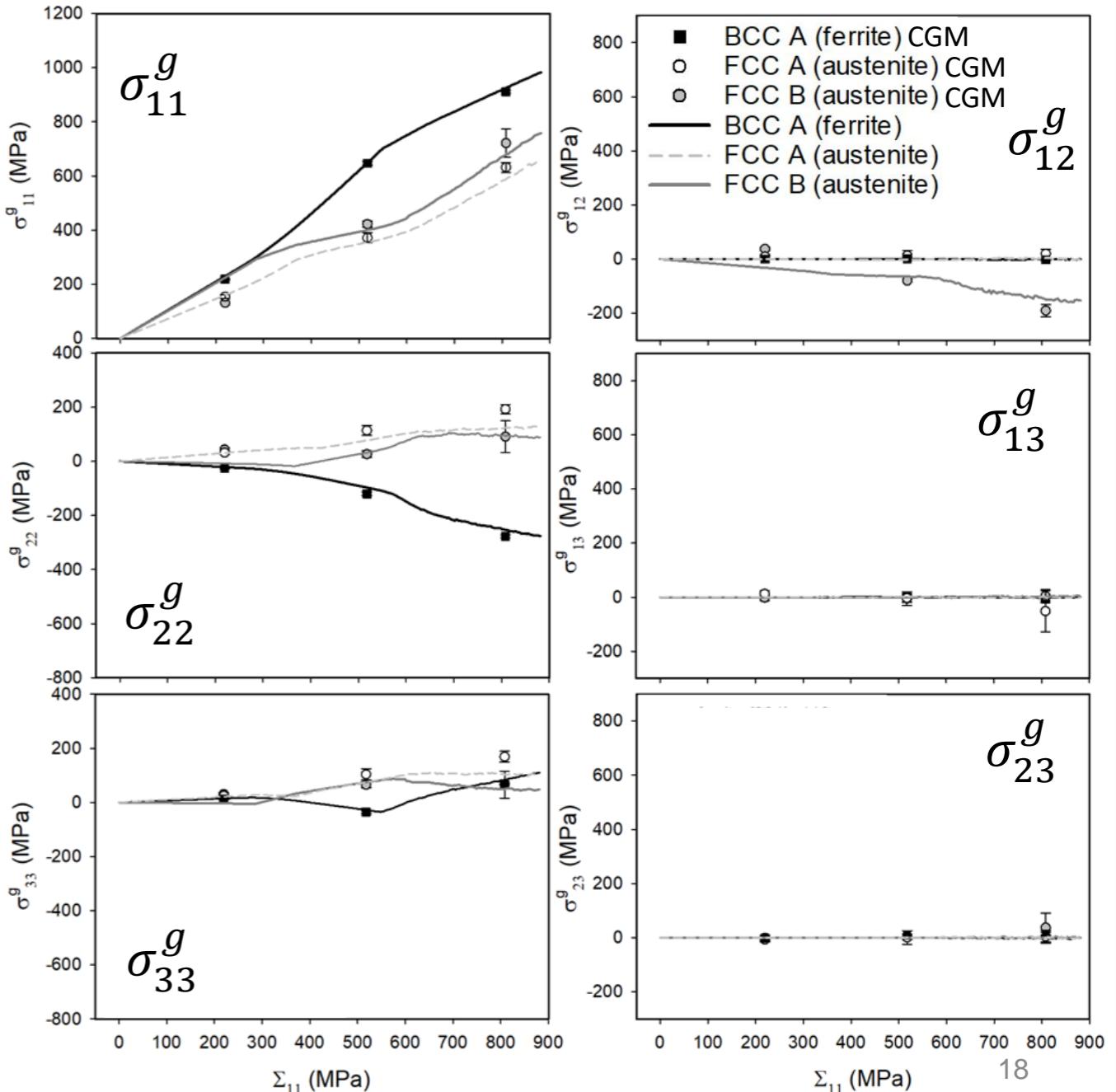
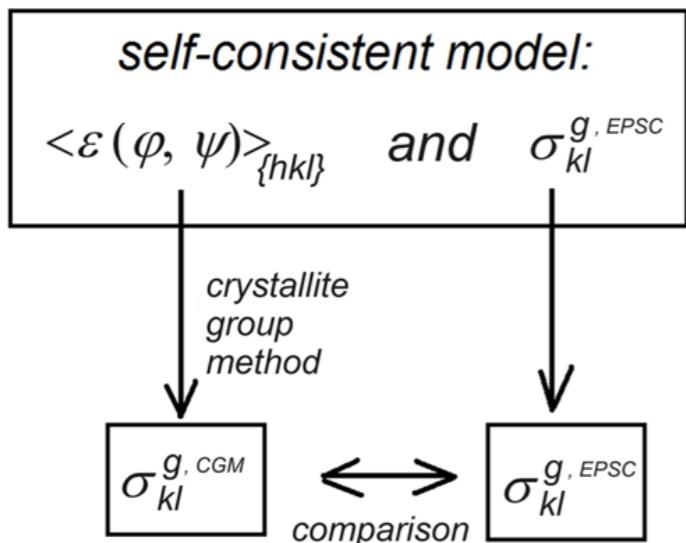
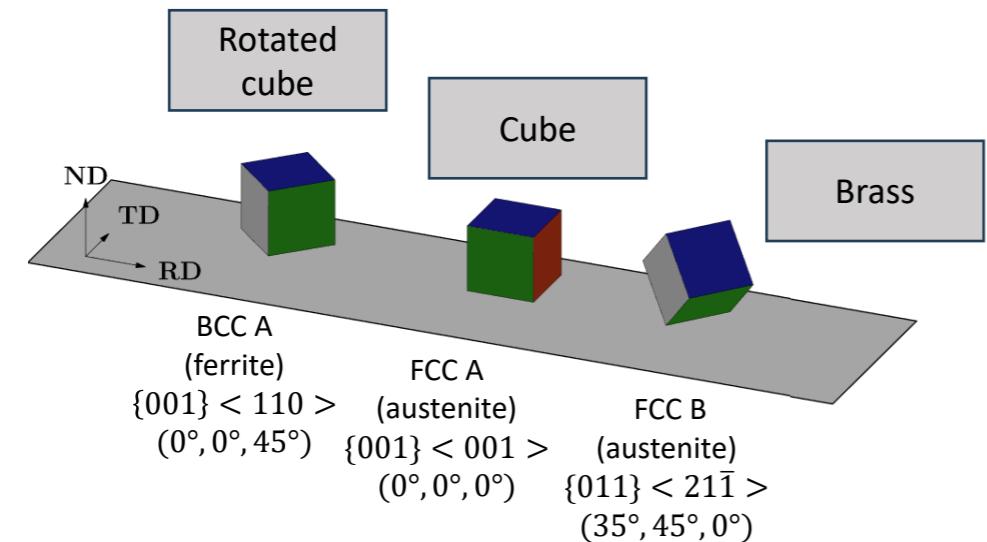
Selection of orientations poles.



Shared poles (for preferred orientations) have to be excluded. Orientations selection should be tested to check if CGM works properly for given texture.



# Crystalite Group Method (CGM) test (duplex steel)

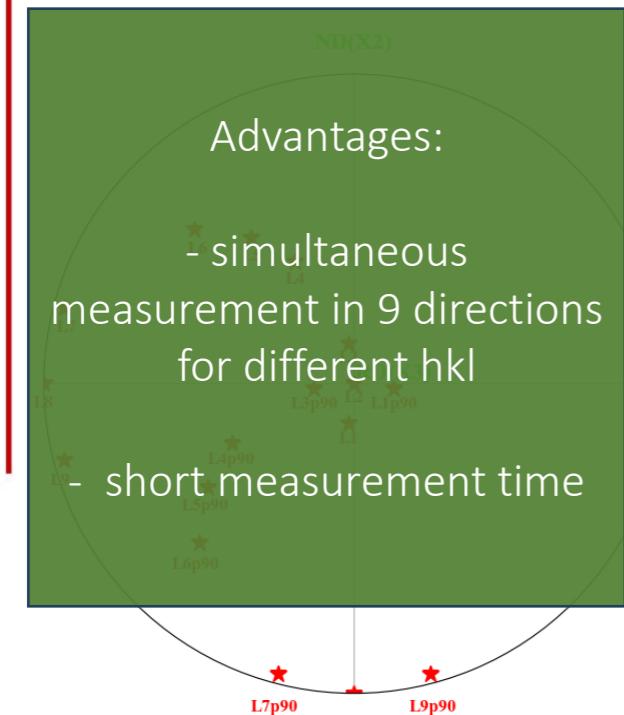


# Measurements Setups

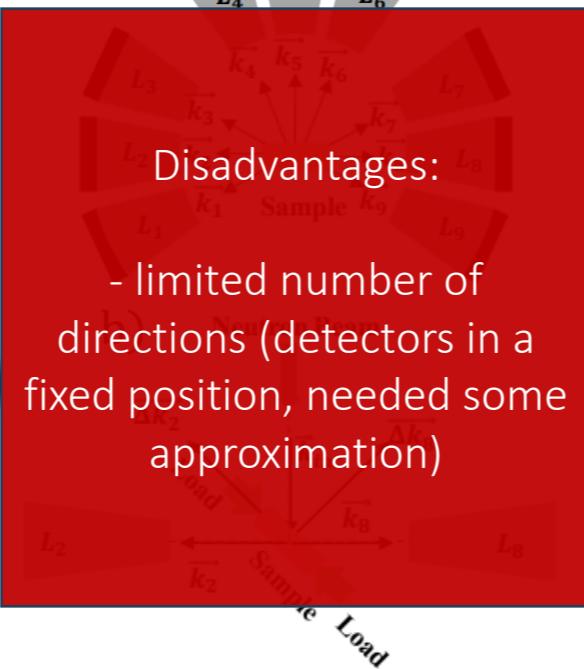
## Two-phase Brass - Time of Flight (ToF)

EPSILON-MDS (JINR, Dubna) diffractometer: 9 detectors, perpendicular to the primary beam

$$d_{hkl} = \frac{ht}{2 \sin \theta m_n L} \quad 2\theta = 90^\circ$$



Poles corresponding to the orientations of the scattering vectors of detectors L1-L9 presented in the sample system  $X$ .

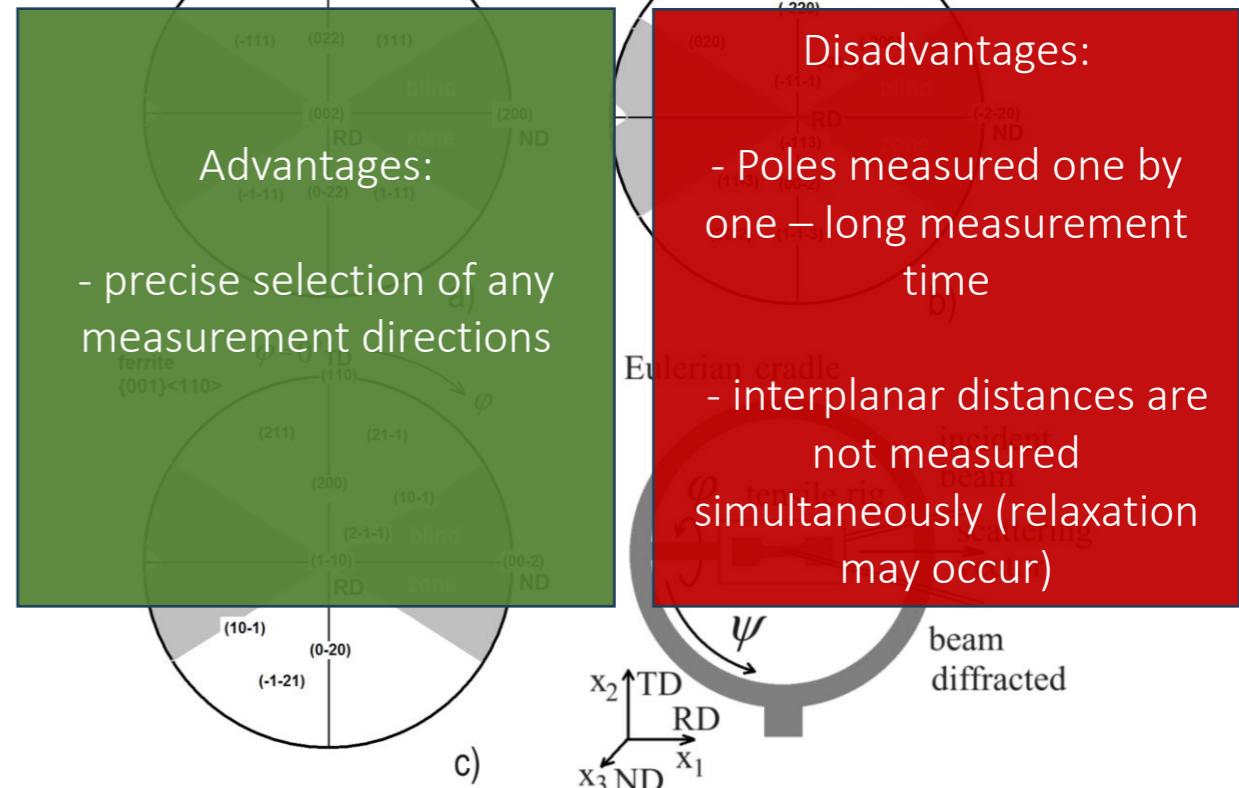


Arrangement of detectors in the EPSILON-MDS diffractometer, a) front view, showing the directions of diffracted beams, b) top view, showing two example scattering vectors  $\Delta k_2$  and  $\Delta k_8$ .

## Duplex steel - angular dispersion

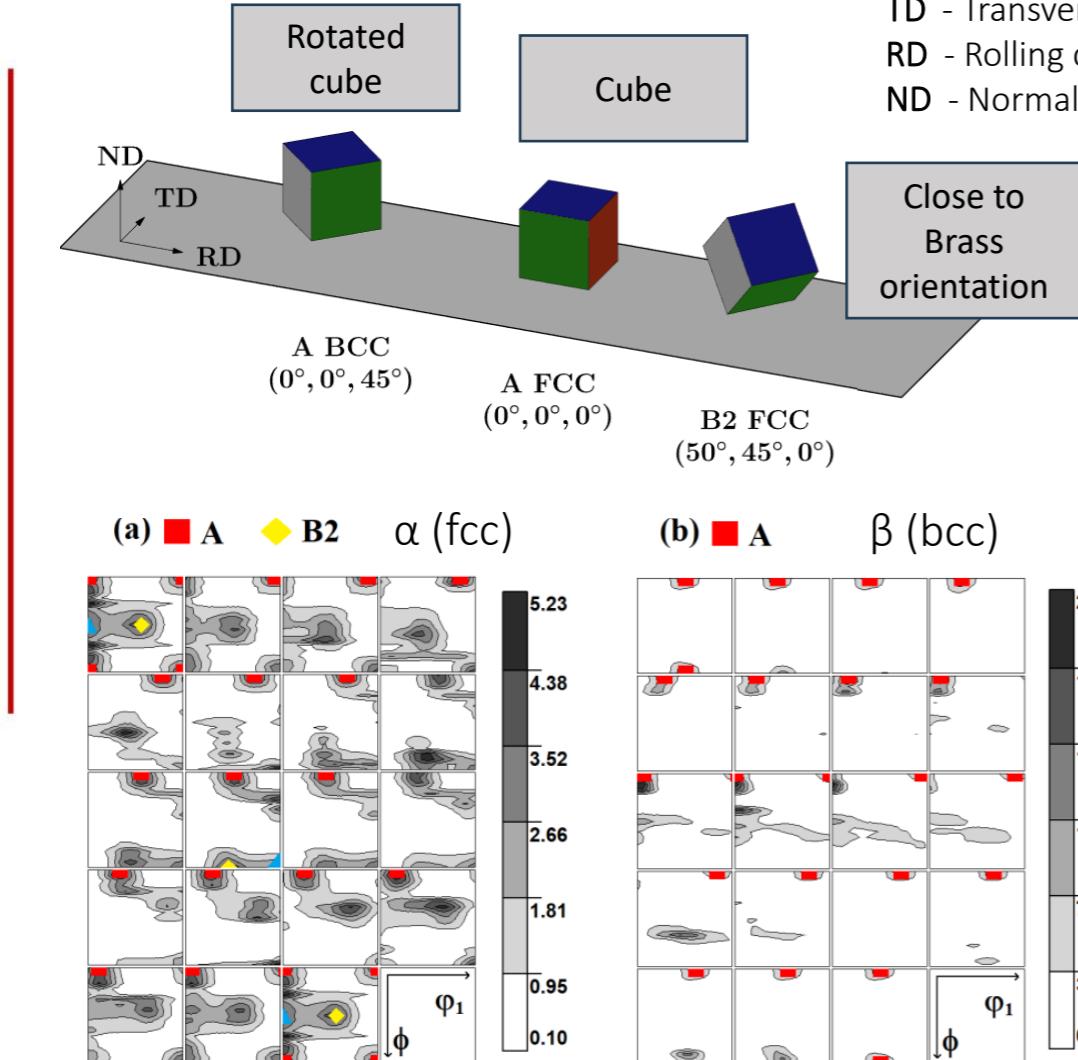
6T1 (LLB, Saclay) diffractometer: 1 detector, Eulerian cradle; Currently measurements done in TKSN400 (NPI, Prague)

$$d_{hkl} = \frac{\lambda}{2 \sin \theta} \quad \lambda = 0,1159 \text{ nm}$$



Poles corresponding to a, b) two preferred orientations in austenite and c) one orientation in ferritic phase. Orientation of the tensile rig (with the sample) rotated in Eulerian cradle is defined by  $\phi$  and  $\psi$  angles (d).

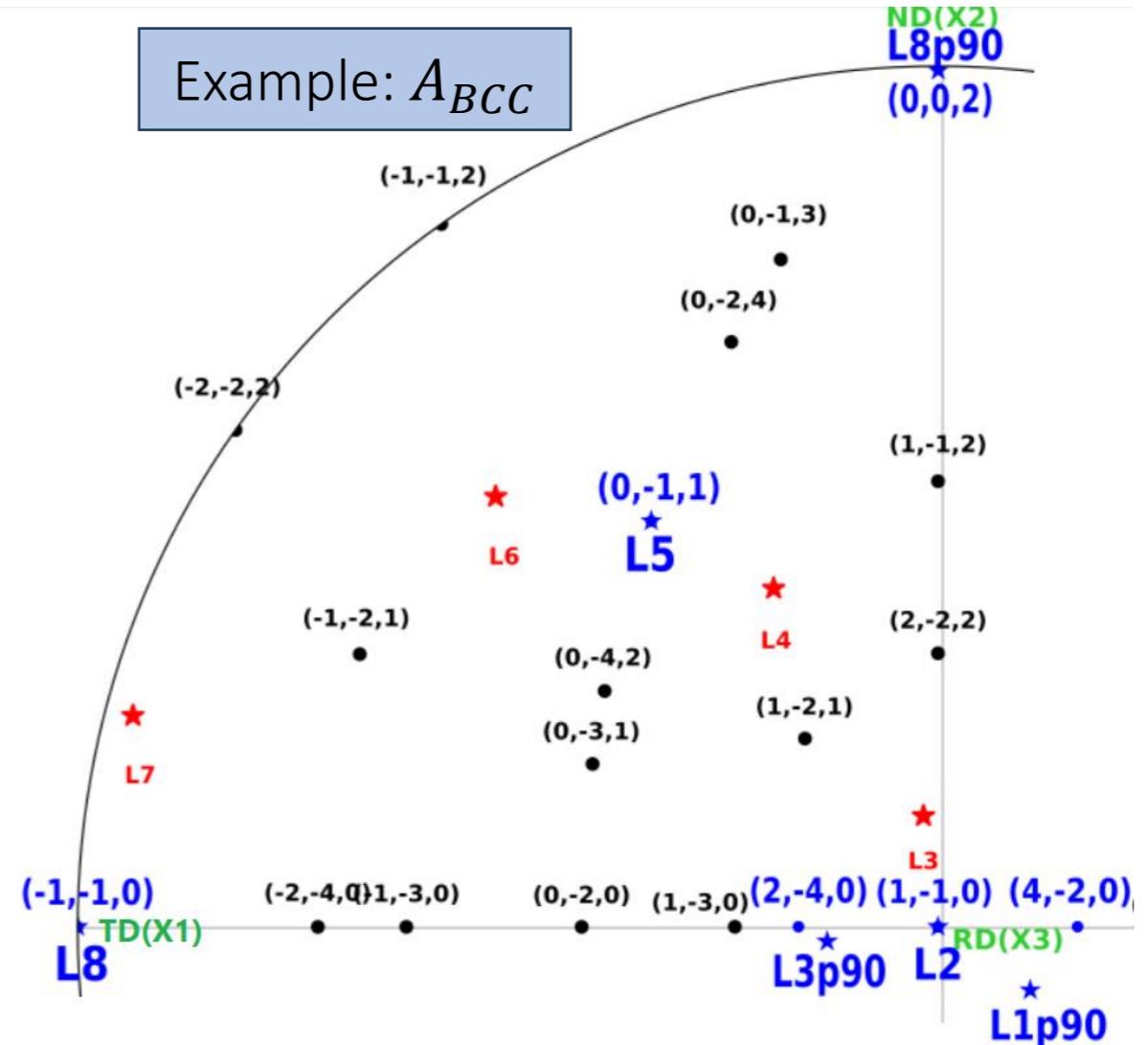
# Brass - Pole Figures Analysis (ToF, CGM)



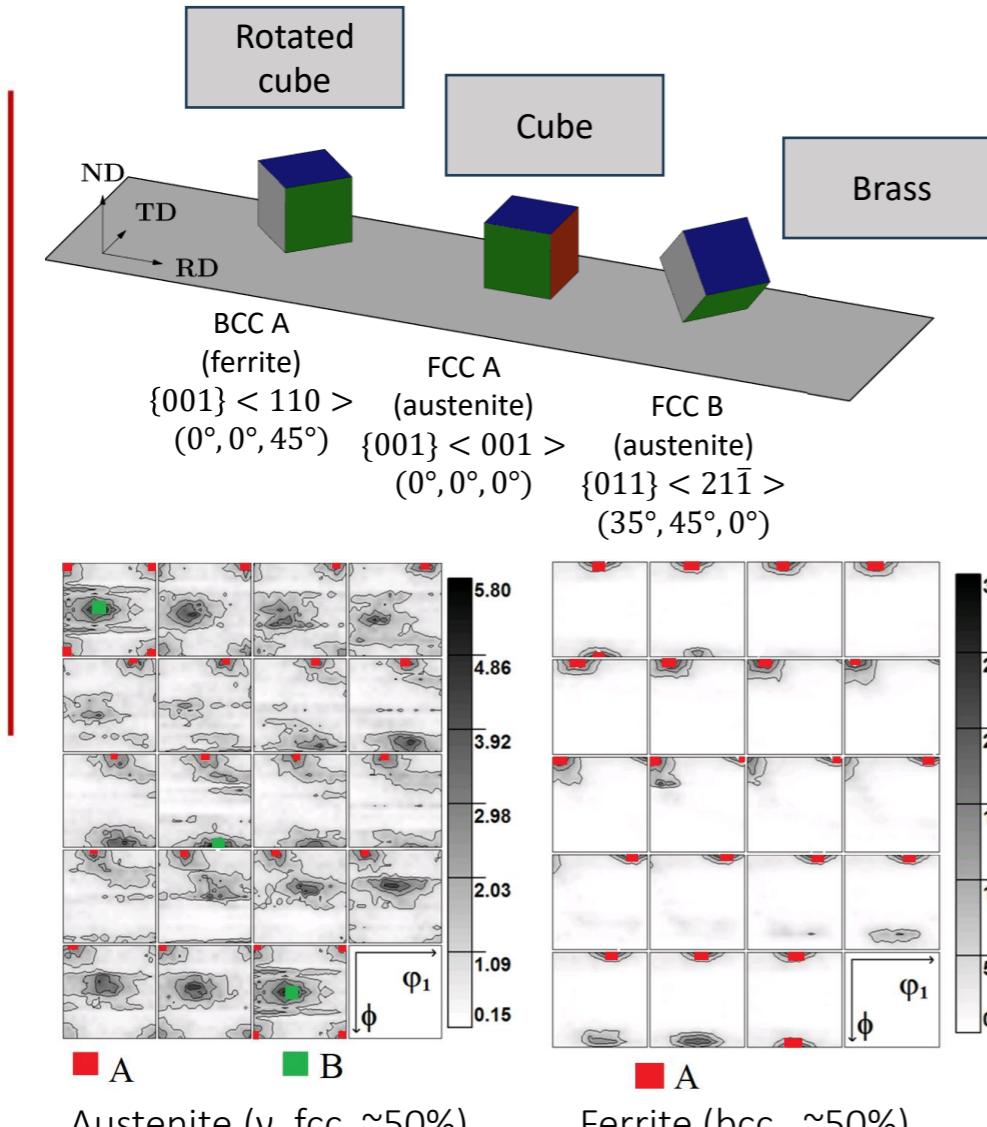
Orientations analyzed for Brass sample.

TD - Transverse direction  
RD - Rolling direction  
ND - Normal direction

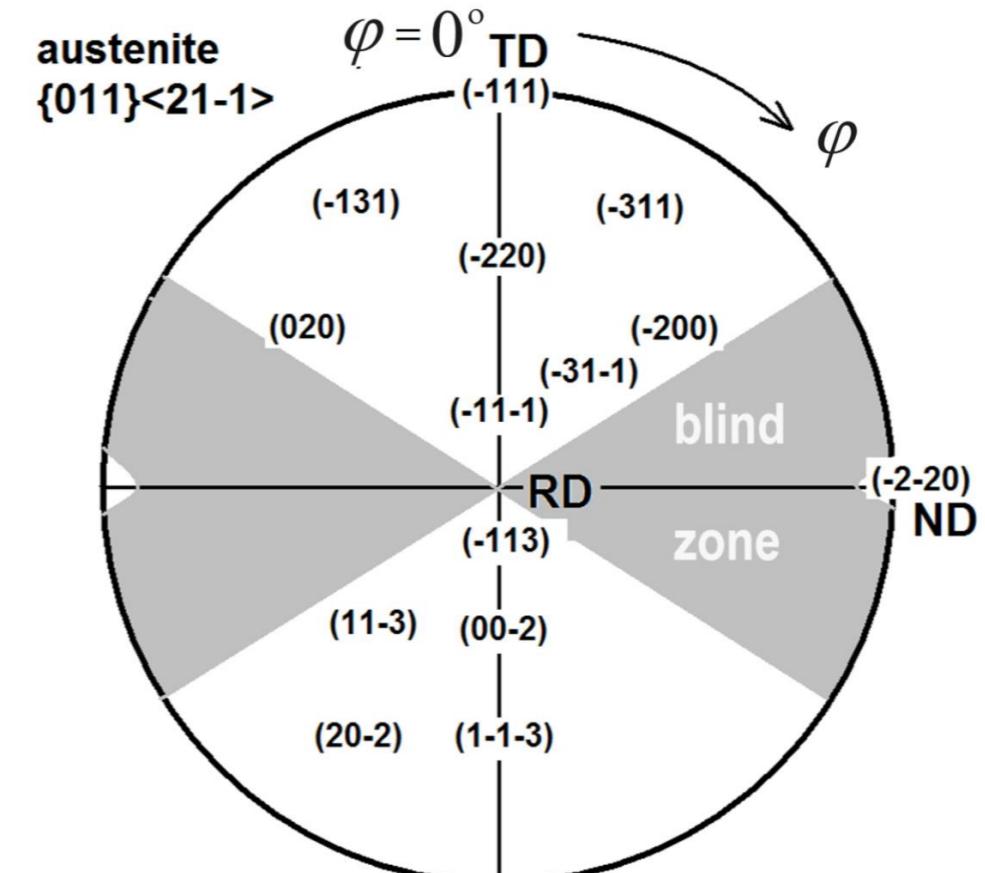
Example:  $A_{BCC}$



# Duplex steel - Pole Figures Analysis (angular dispersion, CGM)



Orientations analyzed for duplex steel.

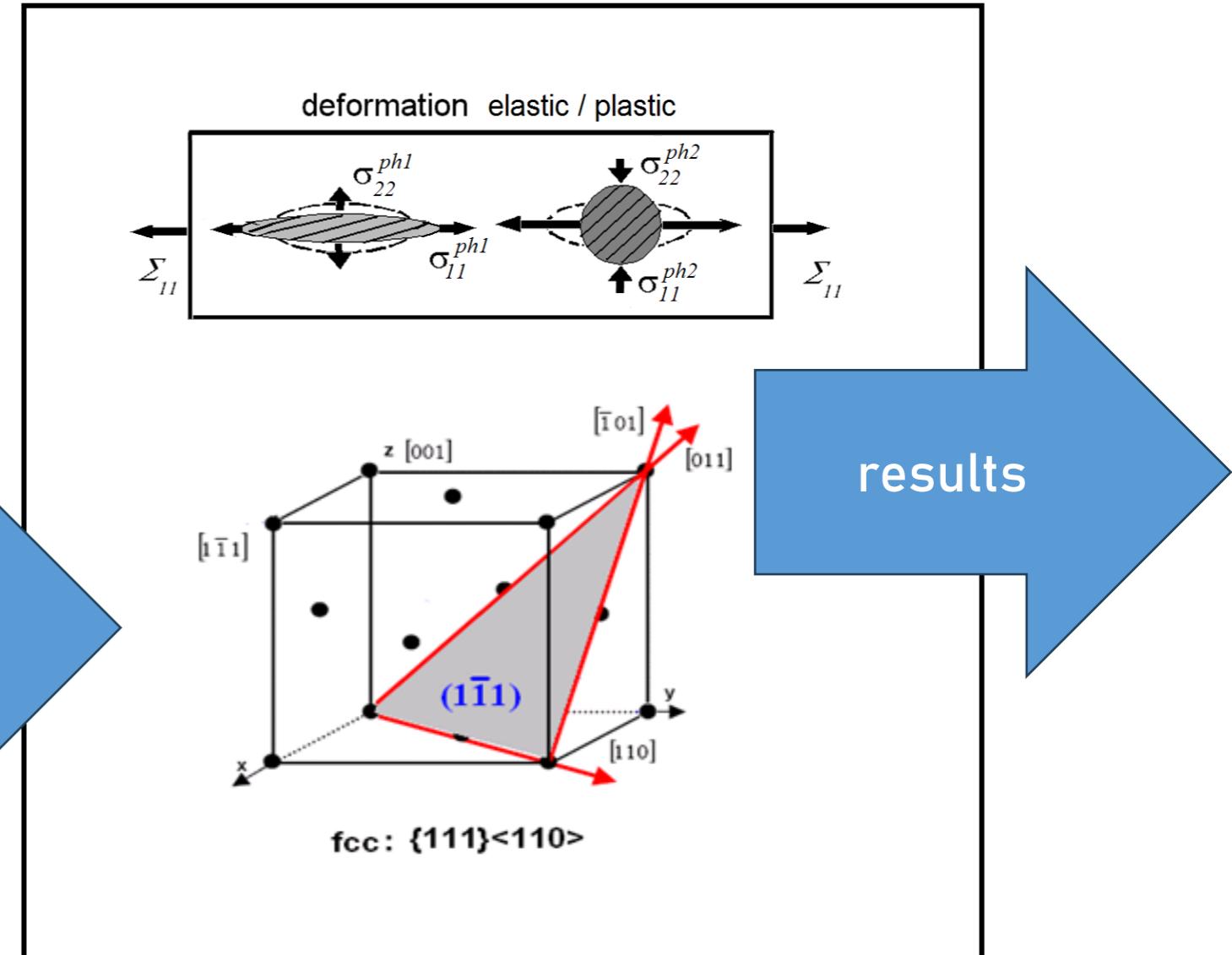


Pole figure for  $B_{FCC}$  orientation with plotted poles corresponding to the scattering vectors orientations set using Eulerian cradle.

# Self-consistent model used for prediction of elasto-plastic deformation

Can we determine  
such parameters as  
CRSS directly from  
diffraction?

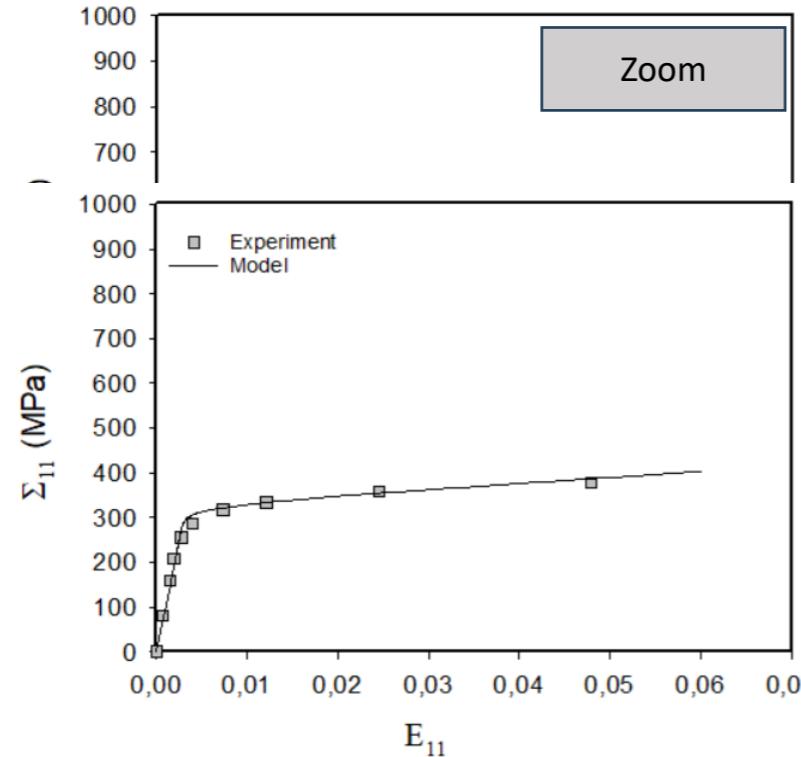
parameters



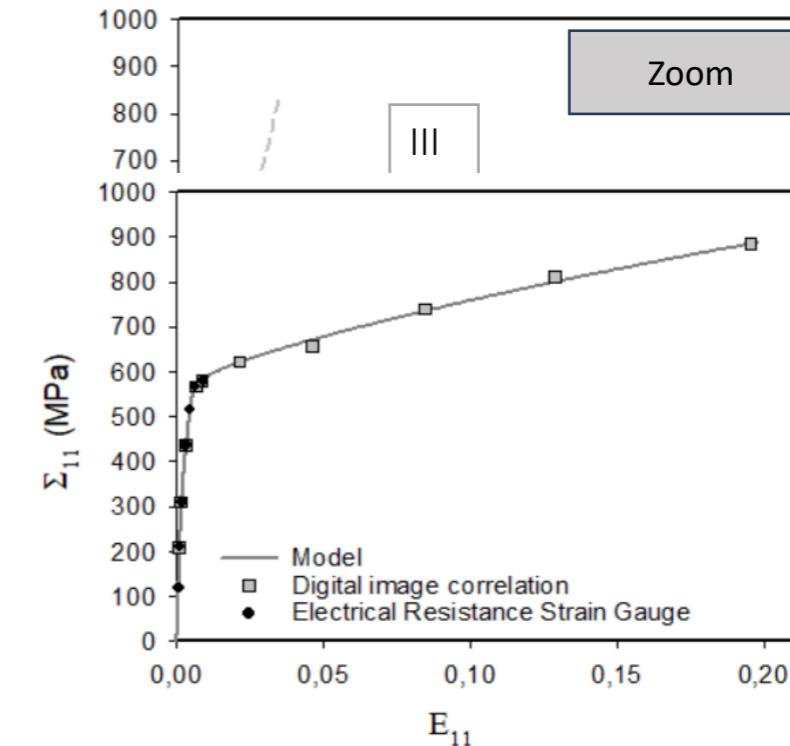
# Macroscopic curves

Measurements performed  
after relaxation

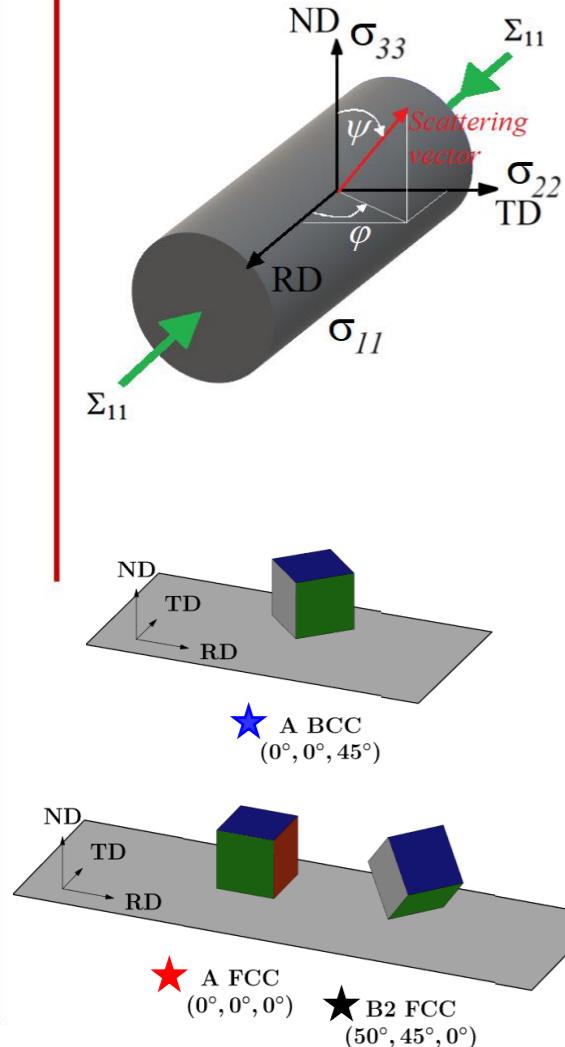
Brass (compression):



Duplex steel (tension):



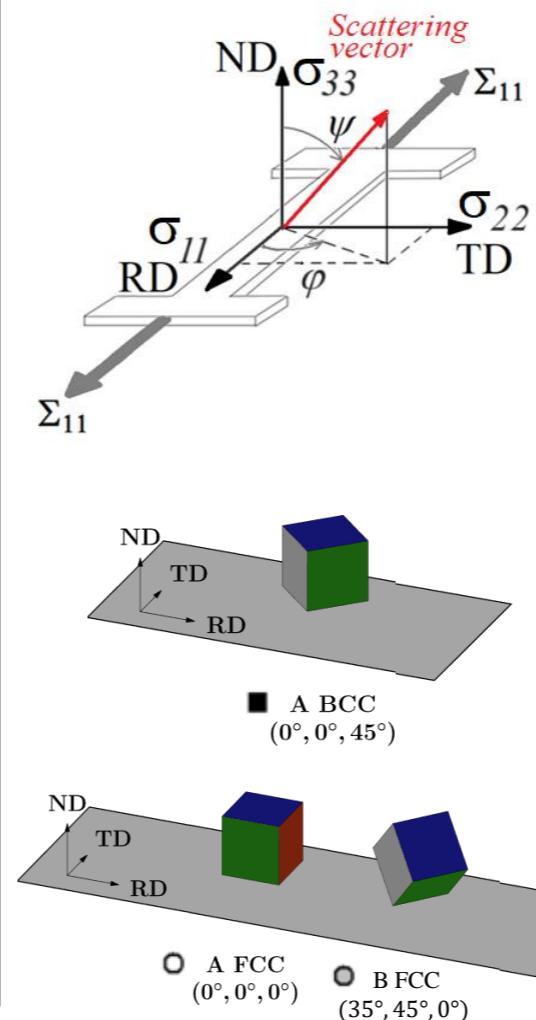
## Brass:



# Normal stresses (CGM)

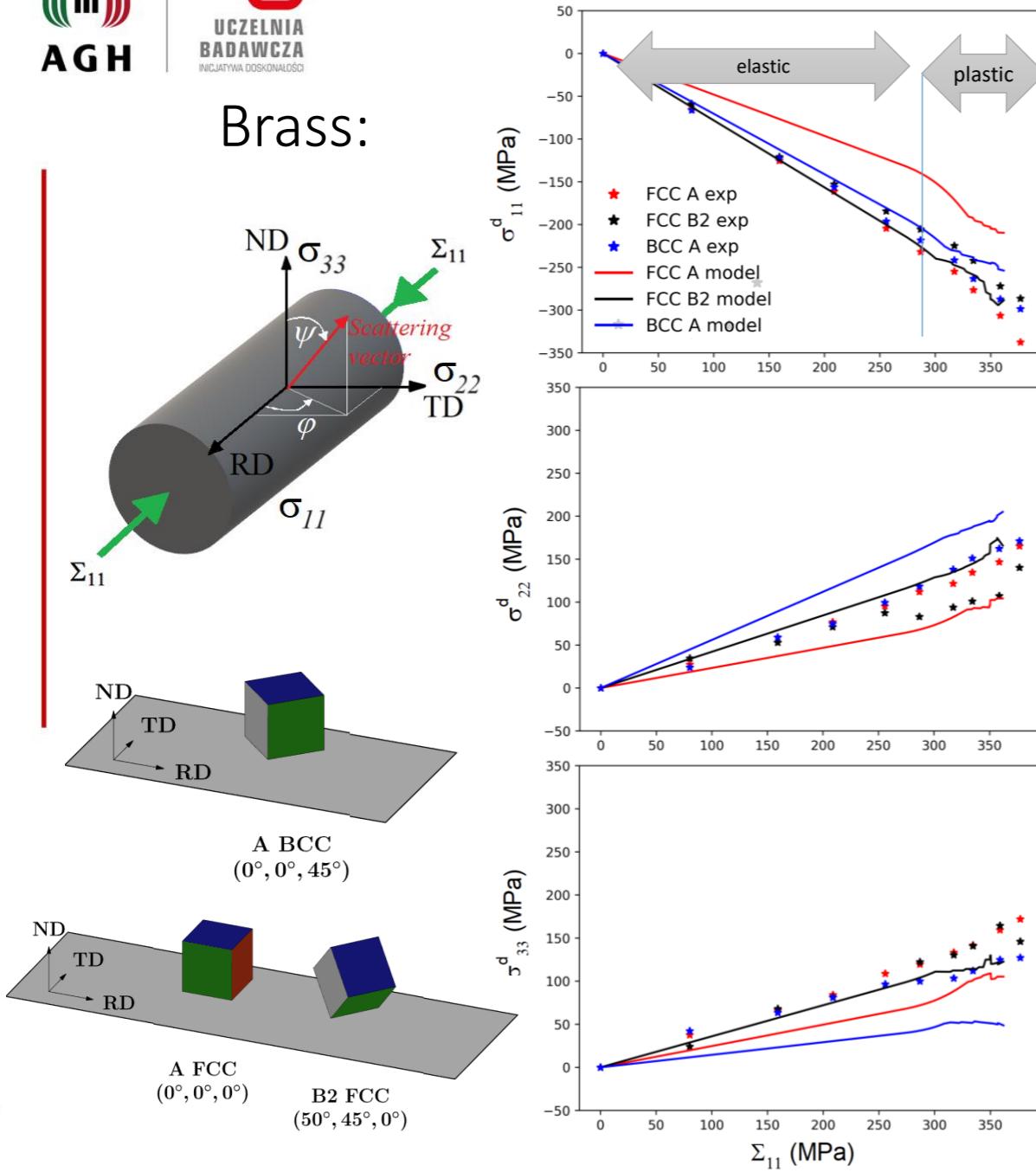
$$\langle \varepsilon(\psi, \phi) \rangle_{\{hkl\}} = a_{3k} a_{3l} s_{kl} l j \sigma_{ij}^{CR}$$

## Duplex steel:

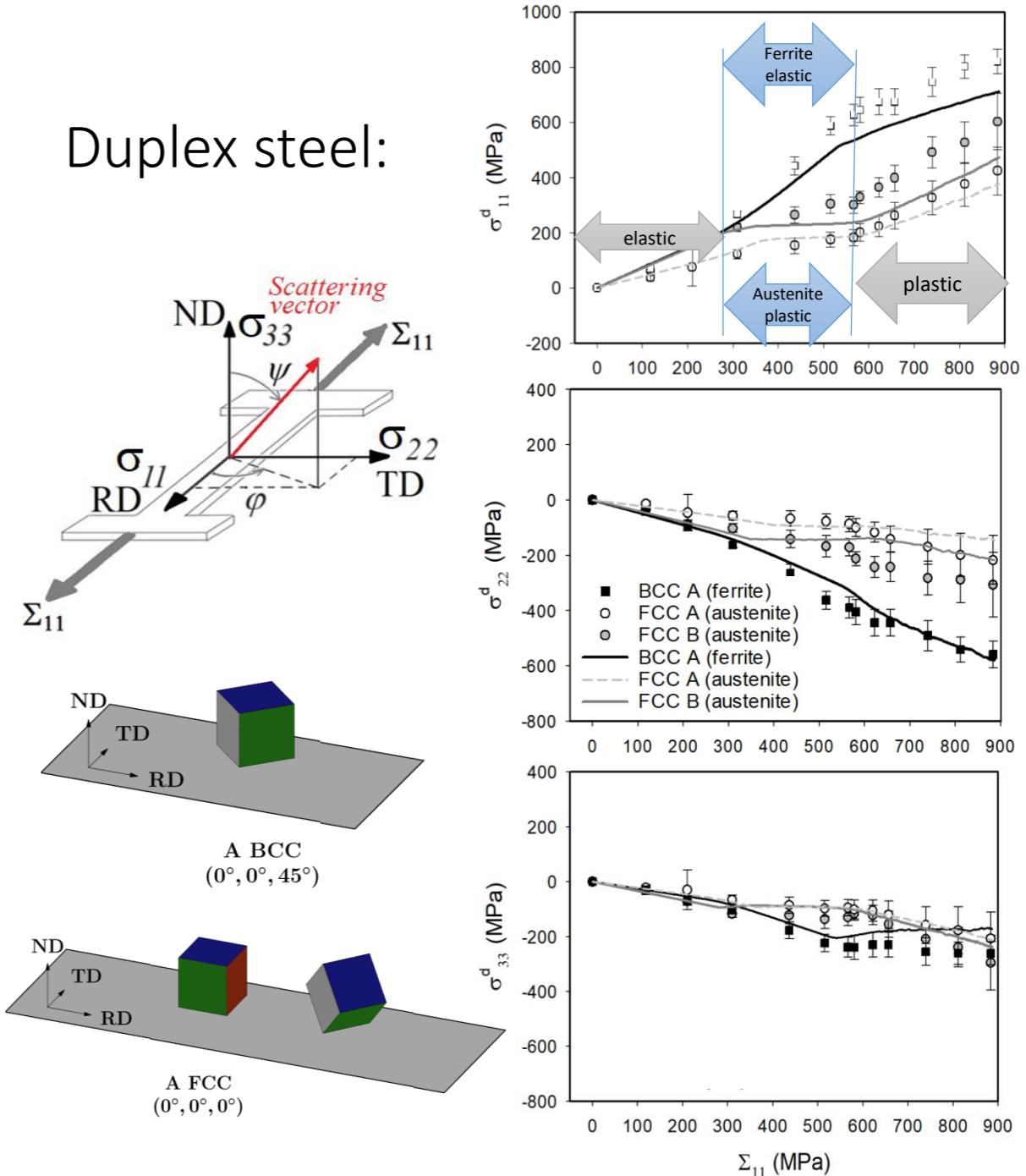


# Deviatoric stresses

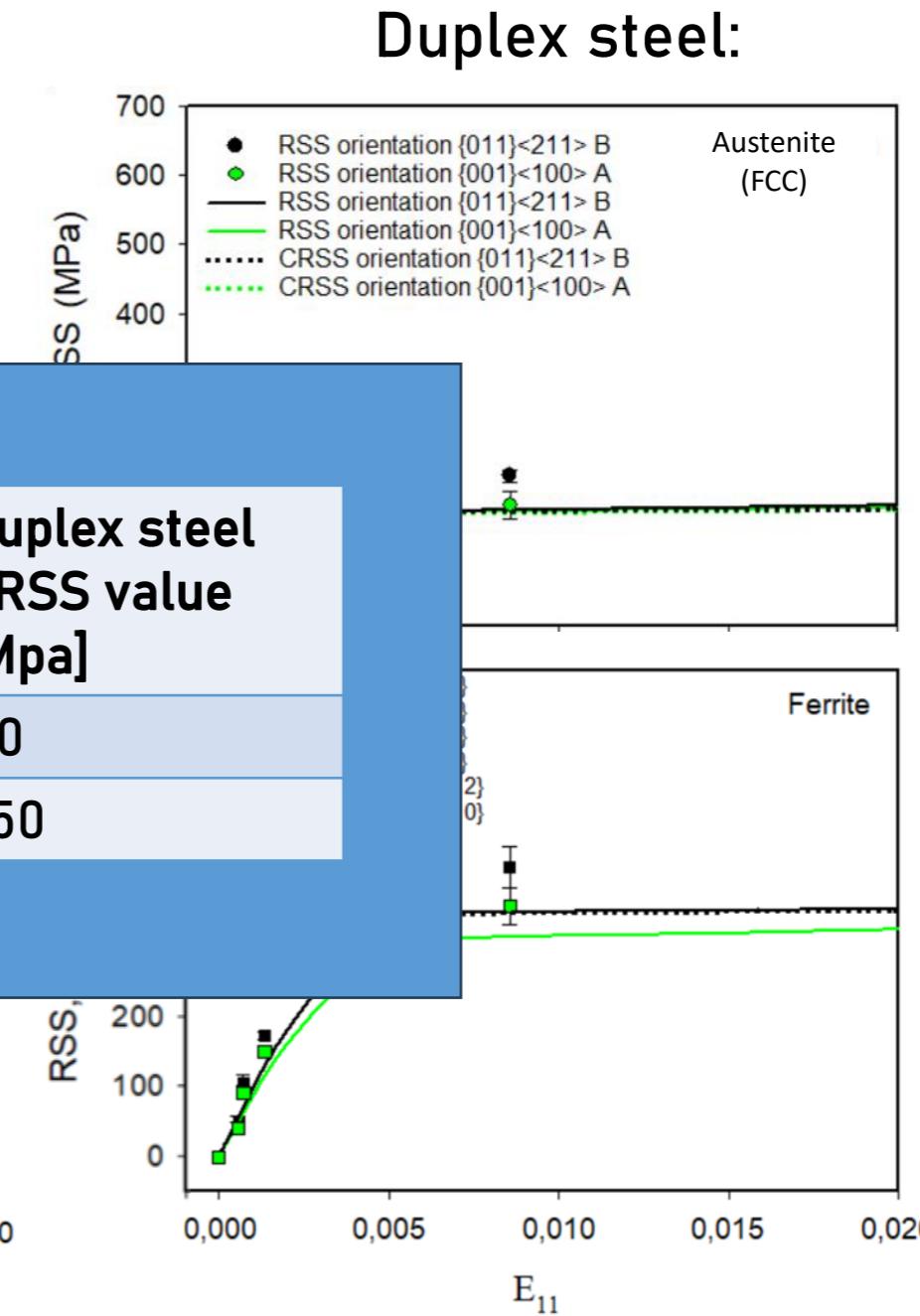
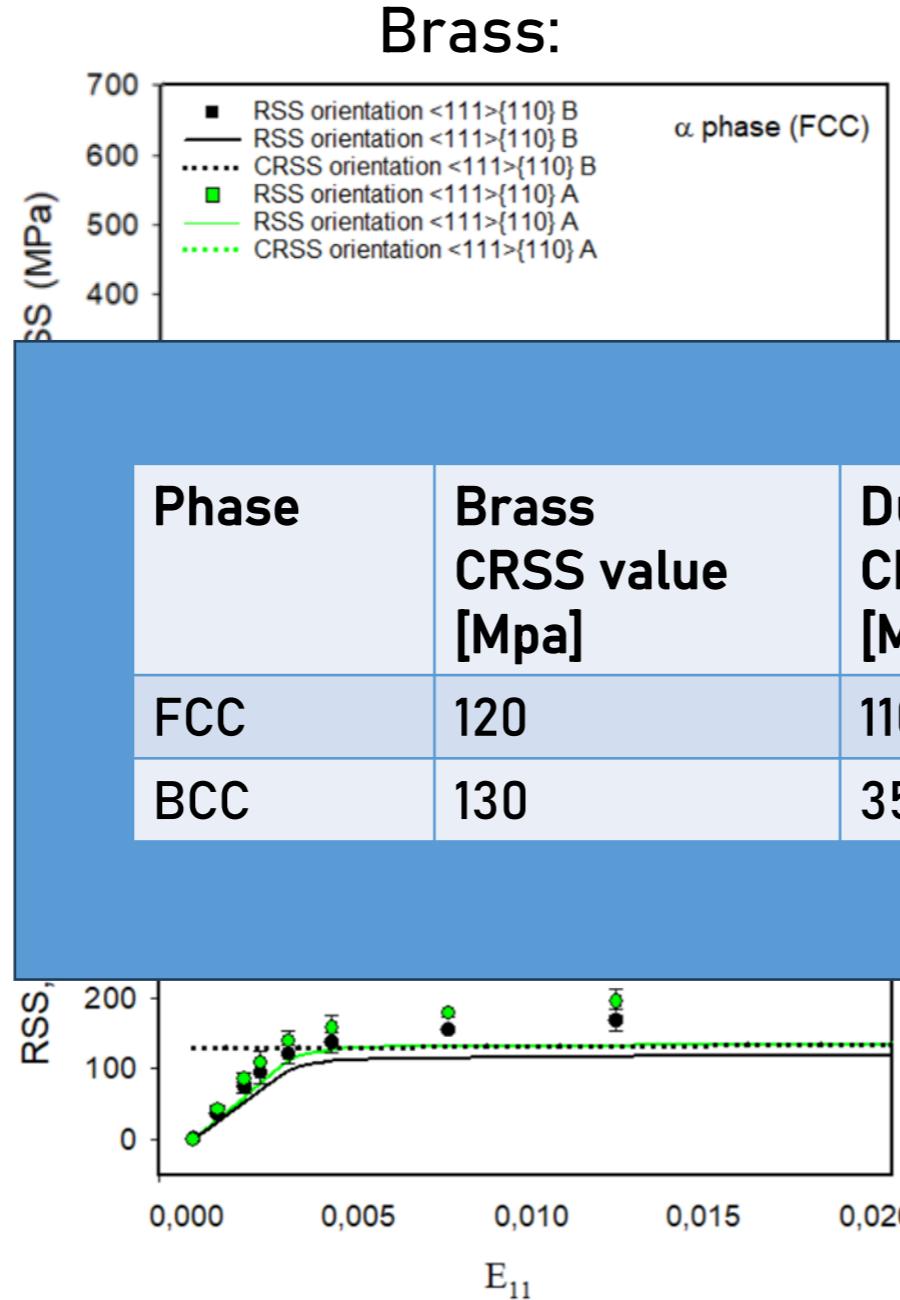
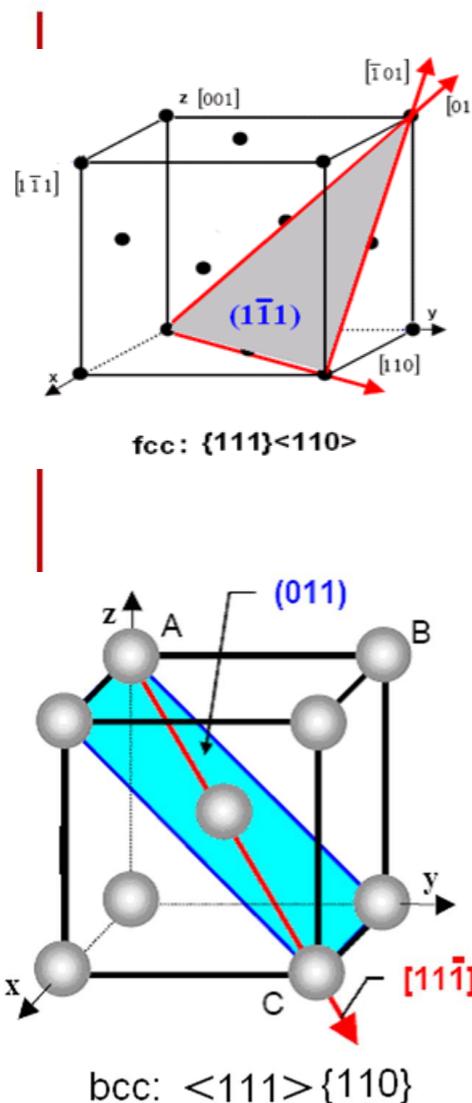
Brass:



Duplex steel:

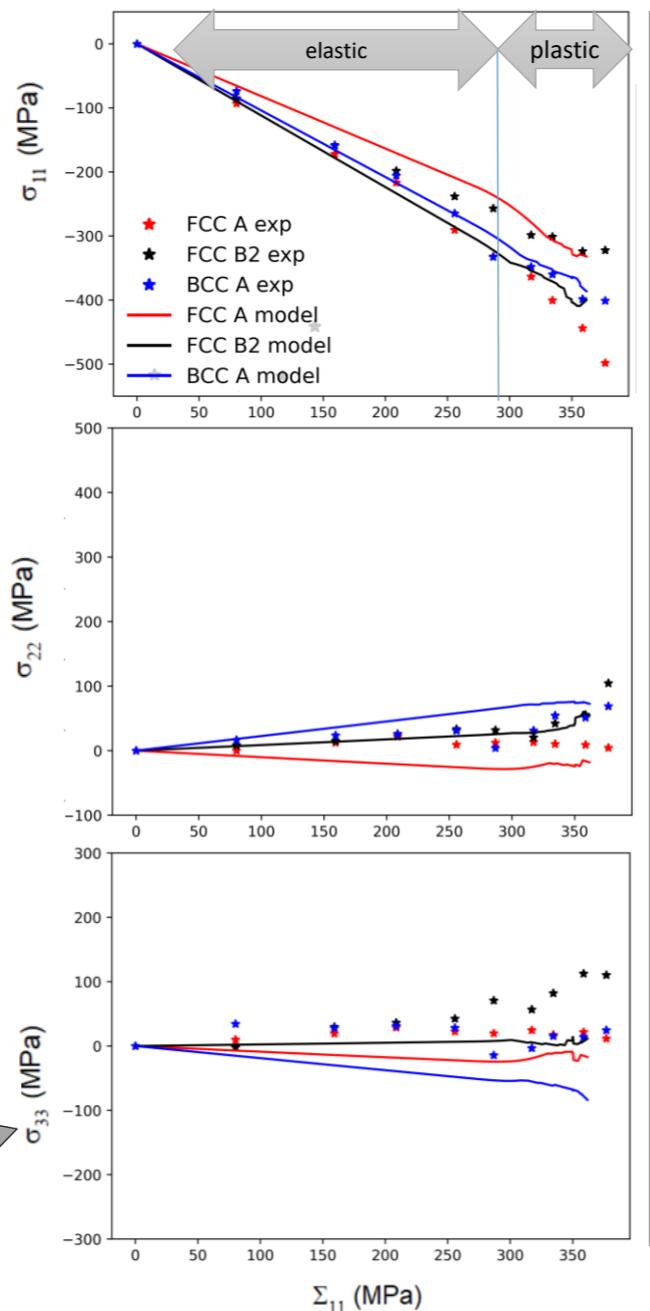
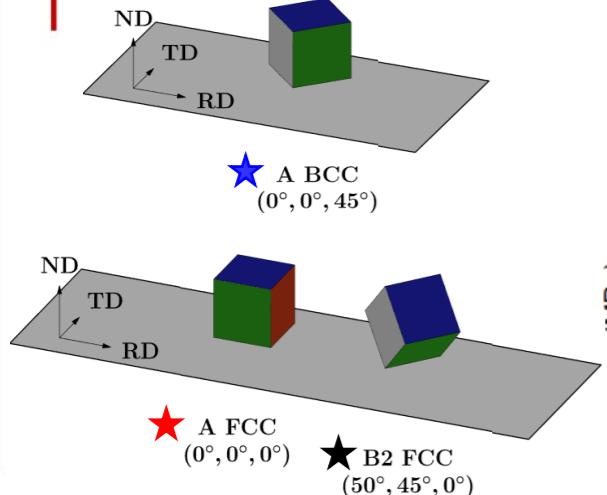
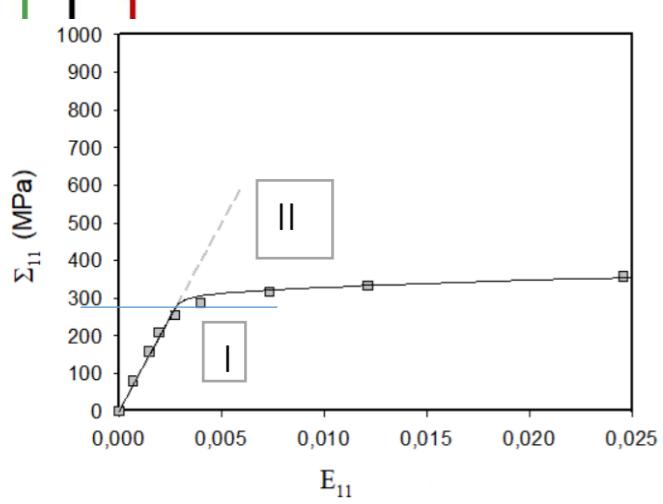


# Resolved Shear Stresses (RSS) + CRSS

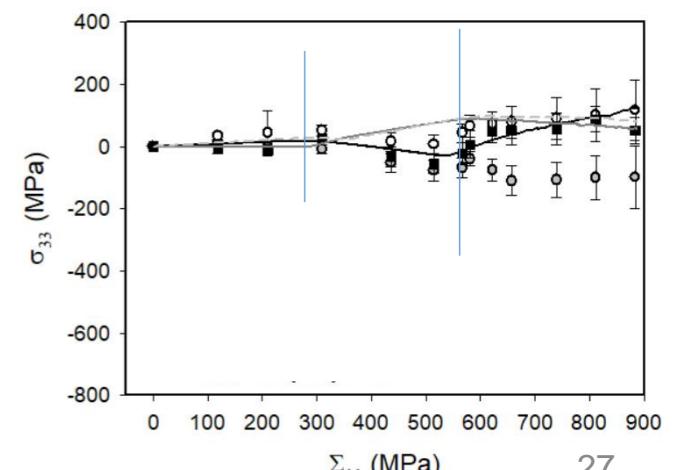
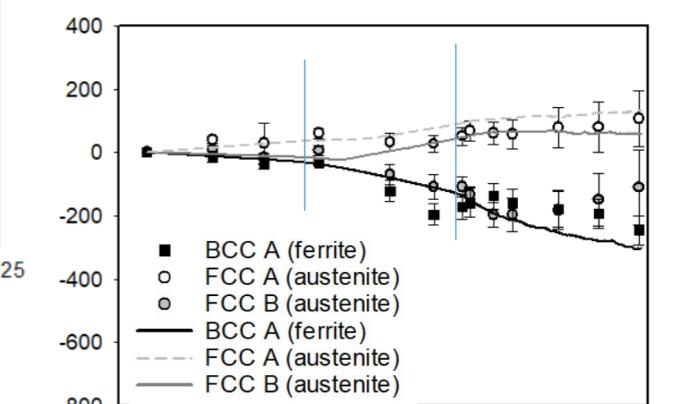
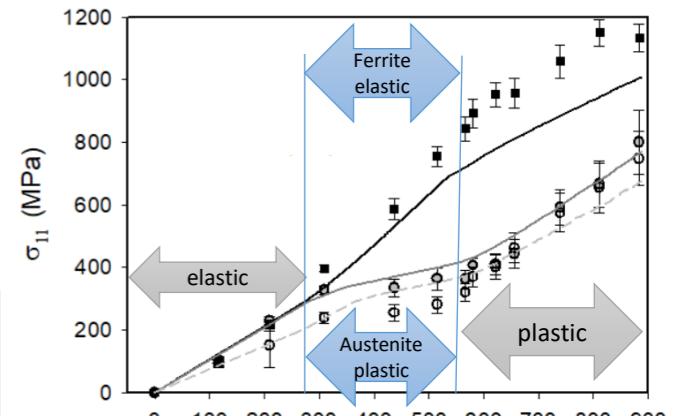
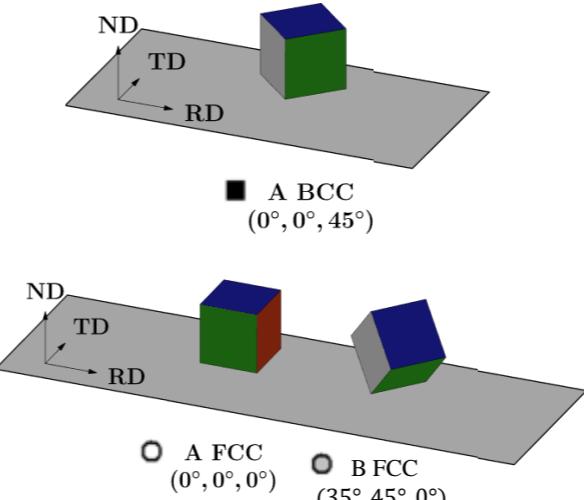
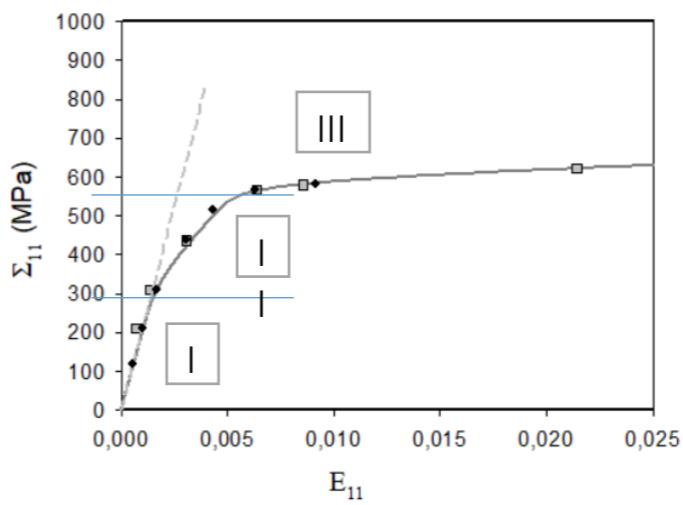


# Results (CGM + model)

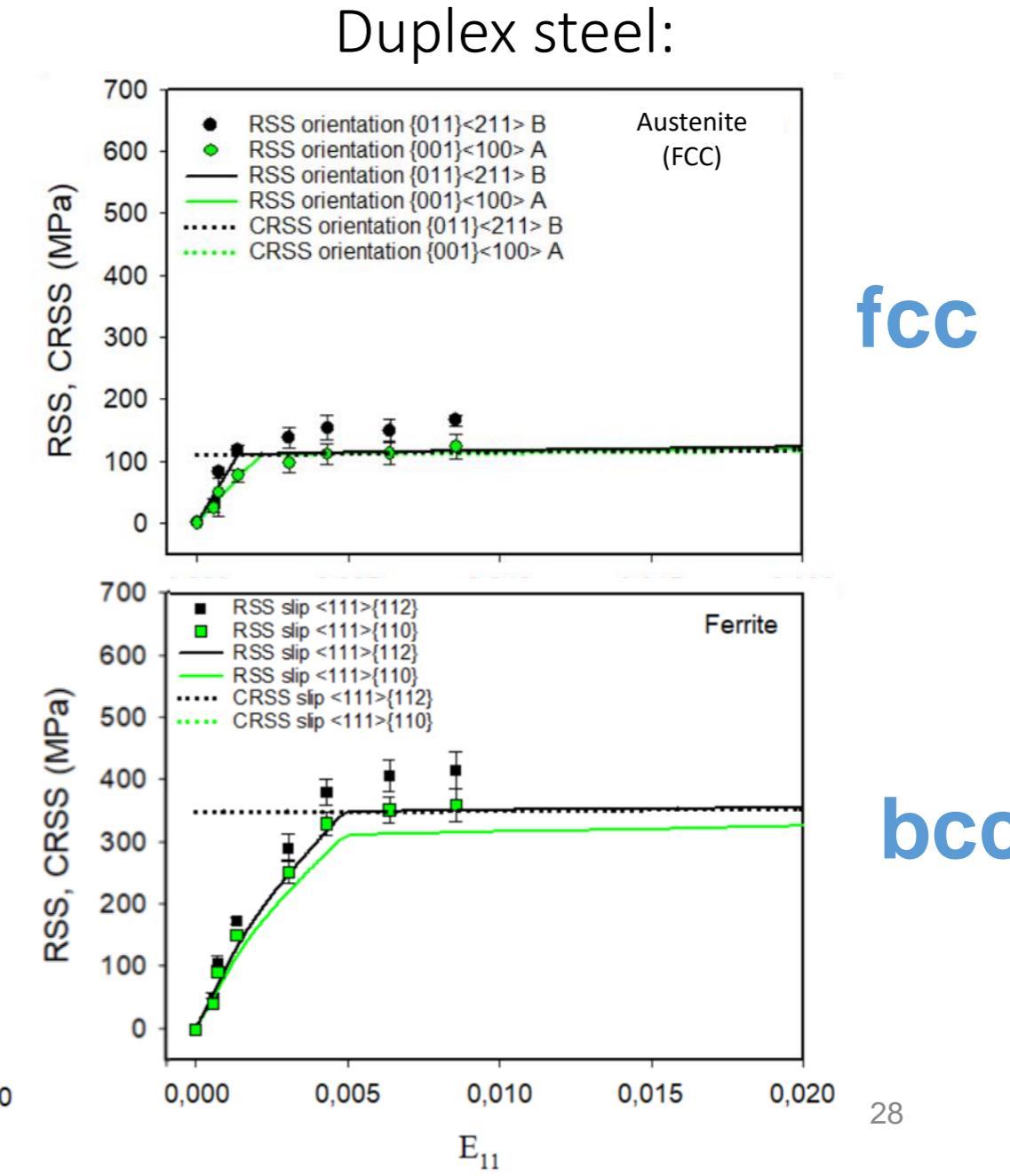
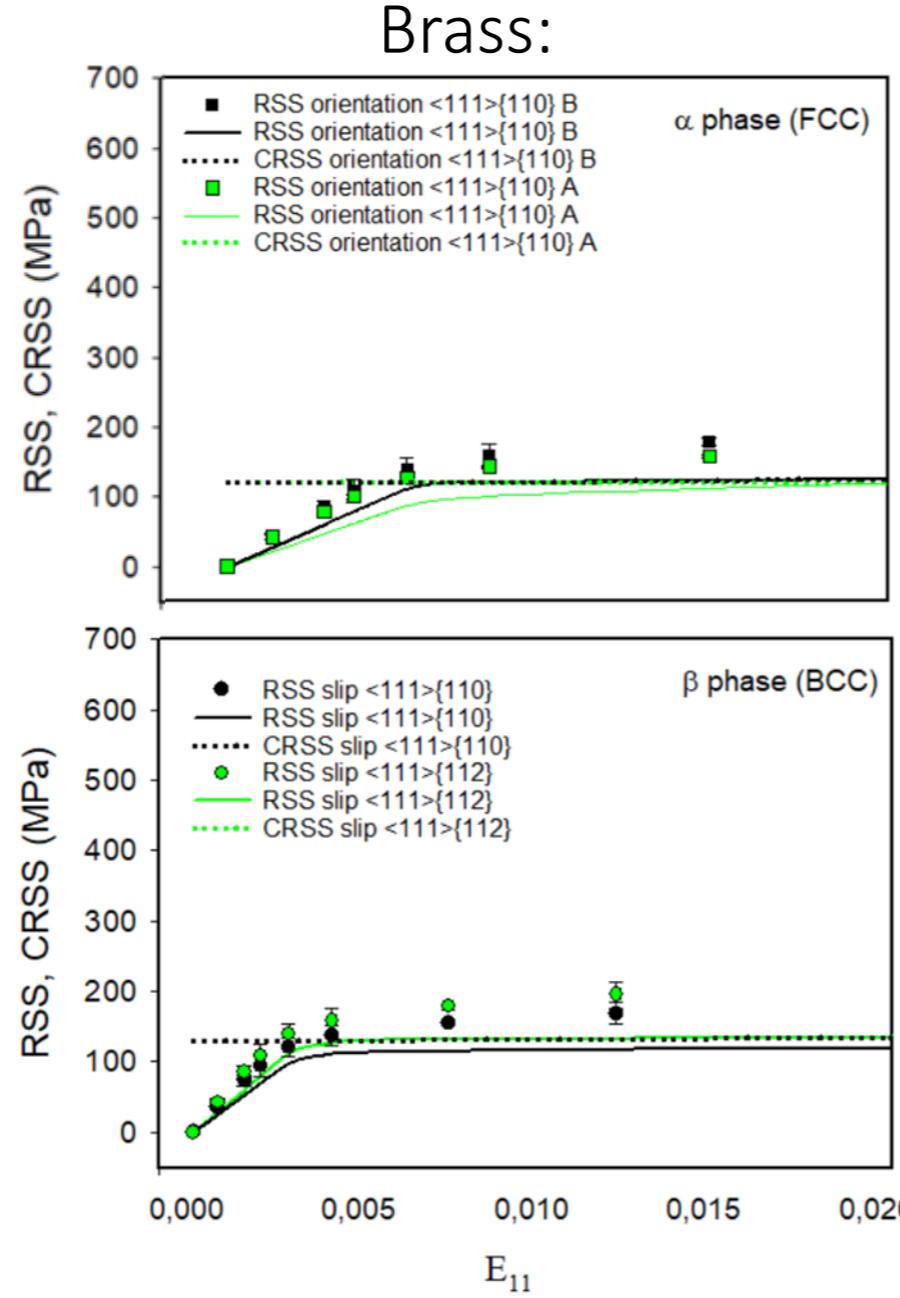
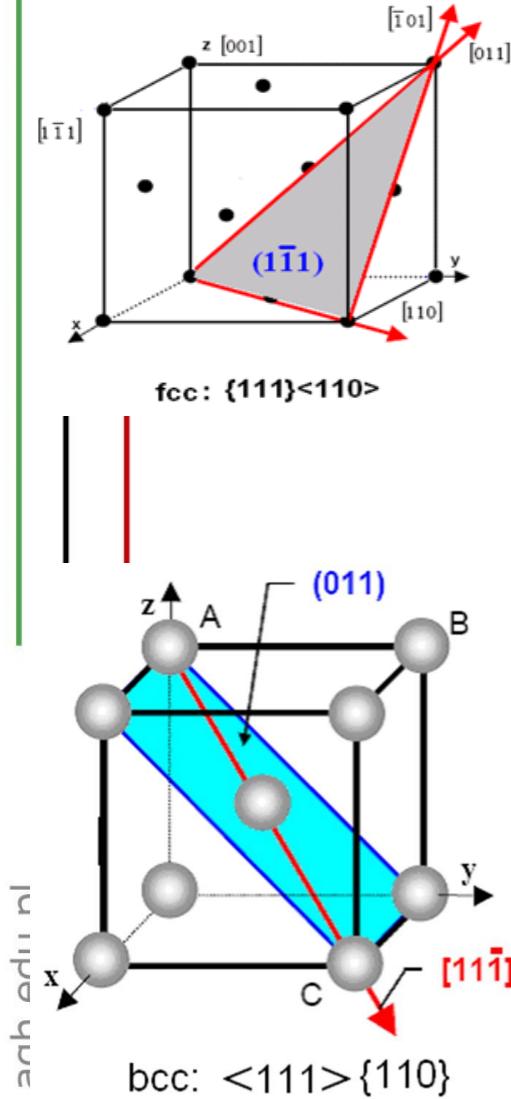
**Brass:**



**Duplex steel:**

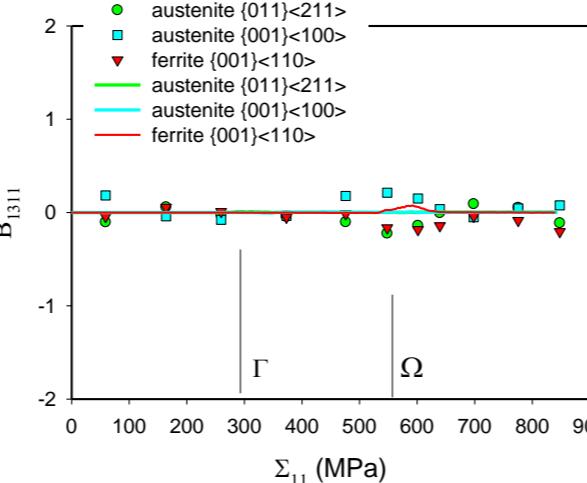
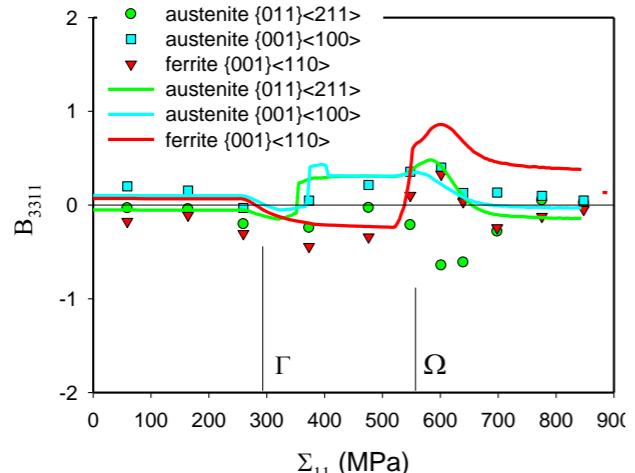
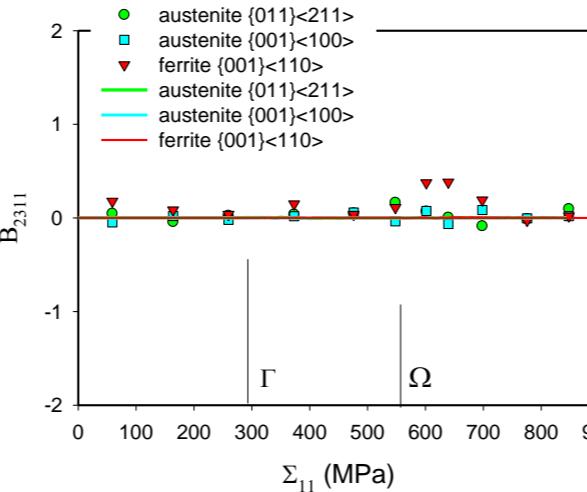
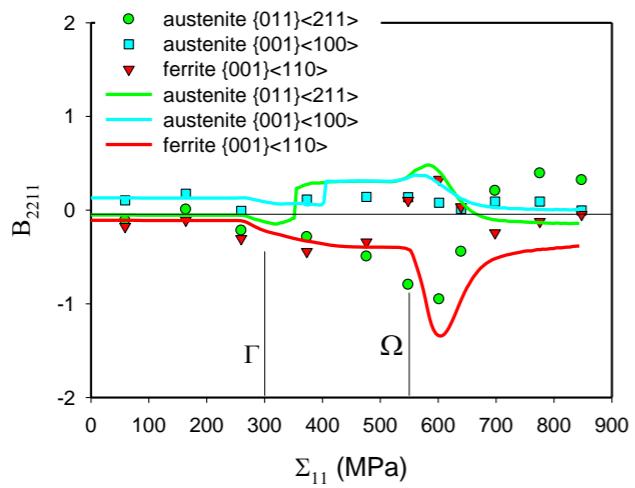
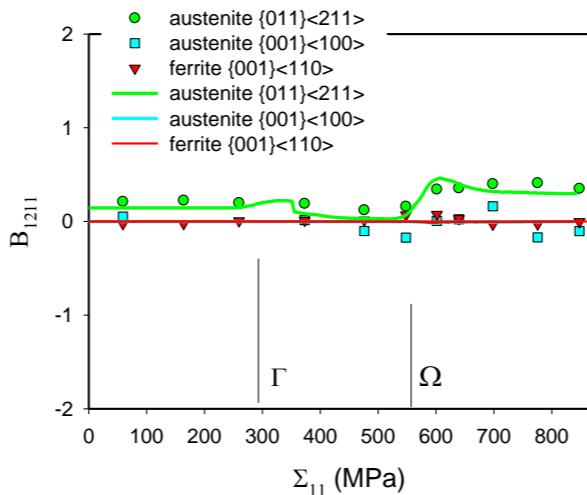
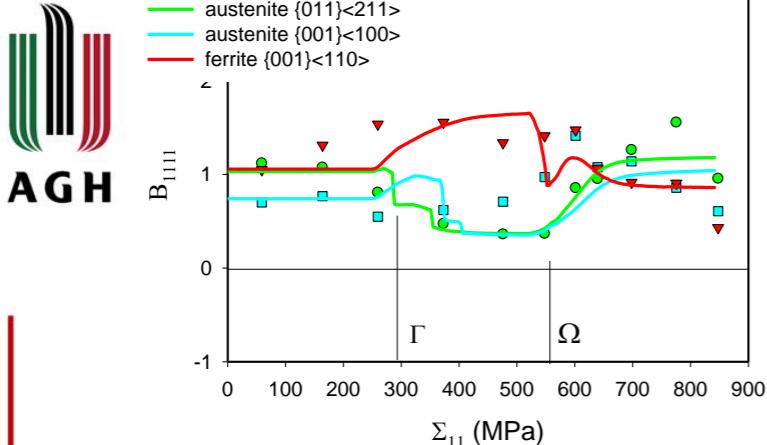


# Resolved Shear Stresses (RSS) + CRSS

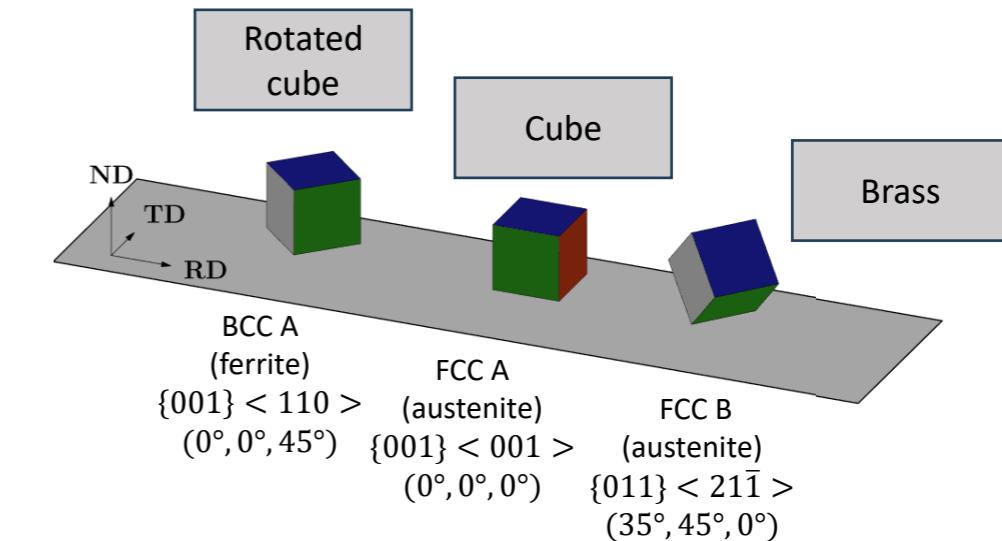


fcc

bcc



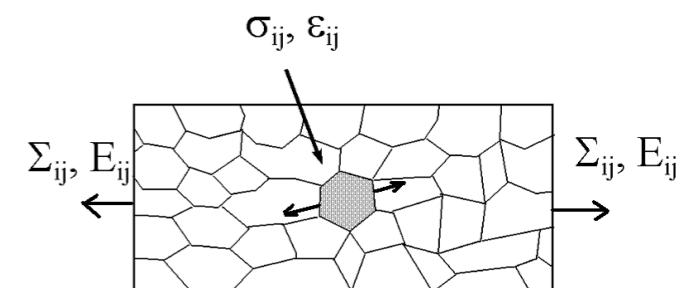
# Stress concentration tensor – duplex steel



Scale transition :

- $\bullet \quad \varepsilon_{ij}^g = A_{ijkl}^g E_{kl}$

- $\bullet \quad \sigma_{ij}^g = B_{ijkl}^g \sum_{kl}$



$\overline{B}_{ijkl}$  model → lines

$B_{ijkl}$  experiment → points

## SUMMARY:

- 1) Elastoplastic deformation in individual phases was studied using diffraction and crystallographic models.*
- 2) Agreement between the results from neutron diffraction and model was obtained.*
- 3) Grain interaction model can be verified using diffraction data.*
- 4) Evolution of stress localization tensor characterizes elastic-plastic transition.*
- 5) Stress tensor for particular groups of grains can be measured using CGM (crystallite group method).*
- 6) Critical resolved stresses (CRSS) can be determined using CGM.*



Thank you for your attention