Change of scale : from the grain to the structure
Changement d'échelle : du grain à la structure

Brigitte Bacroix

LSPM , Laboratoire des Sciences des Matériaux et des Procédés
CNRS – UPR3407, Université Paris 13, France

Some words of warning

- What does « from grain to structure » means ?

  Grain -> Polycristal -> Structure

- Restriction to plasticity of (poly)crystalline materials.

- Initially a key point for metallurgists; then, strong development of models in mechanics of materials and of « multi-scale » experimental tools.

- Strong multidisciplinarity ; mechanics of materials, mechanical metallurgy

Some important steps

- Plasticity of metals

  Tresca criterion (1864), von Mises criterion (1913),

  Taylor hardening law for fcc metals (1934)

  Anisotropic criterion, Hill (1948), ….

- Crystalline Plasticity

  RX and Bragg (1912), dislocations and TEM observation (Volterra 1905, dislocations in crystal by Frank, 1st microscope in 1930, ….)

  Dislocations by Friedel (1964), Plasticity of Metals by Jaoul (1965)

- Material = Isotropic polycrystal

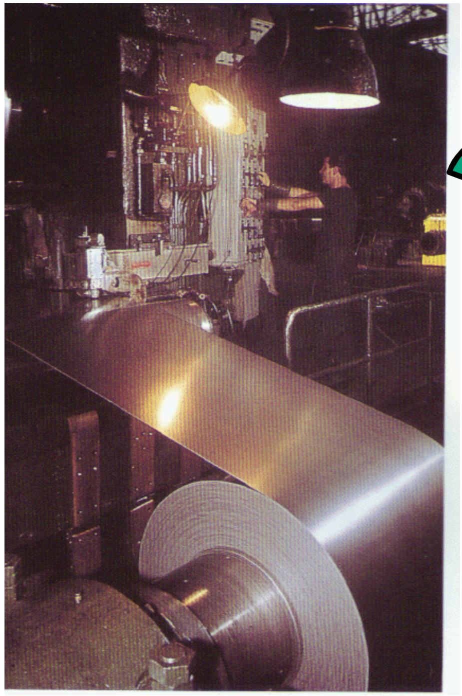
  Sachs (1928), Taylor (1938)

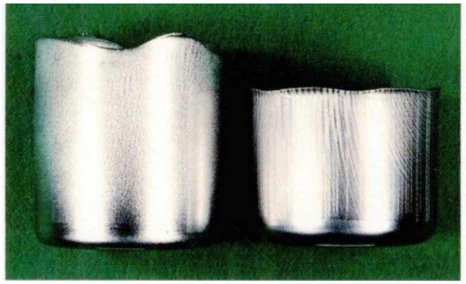
And since then , micromechanics approaches and FE simulations

Introduction

➢ All metals are subjected to complex thermomechanical treatments during the elaboration of semi-products (like sheets) or their transformation into final products (like beverage can)

➢Thermomechanical treatment = plastic deformation, recristallisation, phase transformation

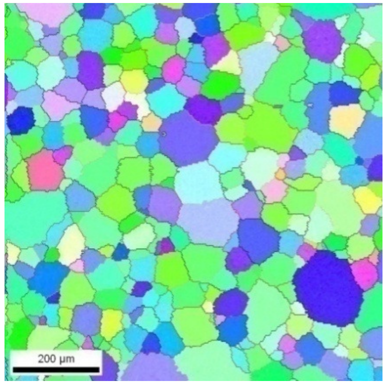


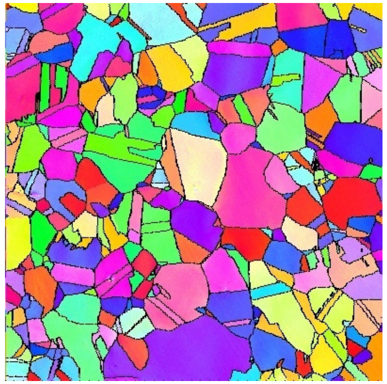


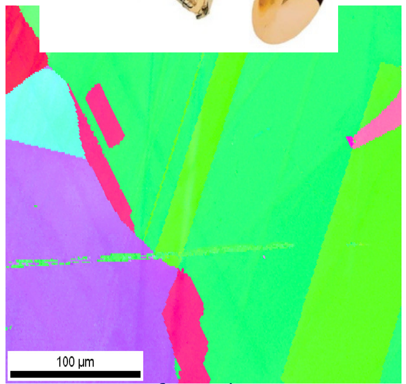
➢ Understand, model and predict what happens during deformation

Introduction

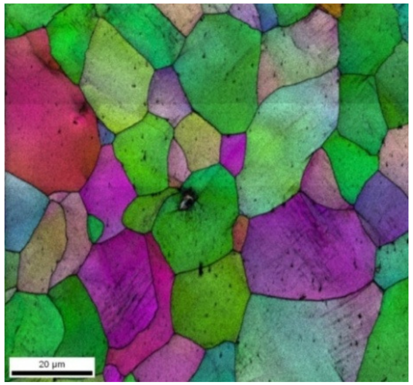
- All steps => strong evolution of texture and microstructure
  => anisotropy of final mechanical properties



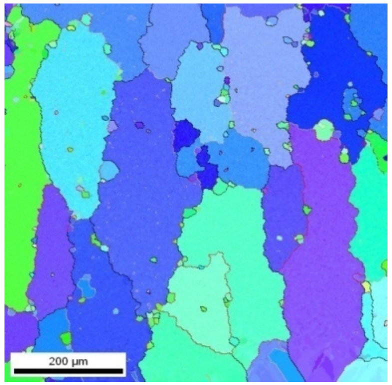




Microstructure of wind instruments
ANR Project CAGIMA

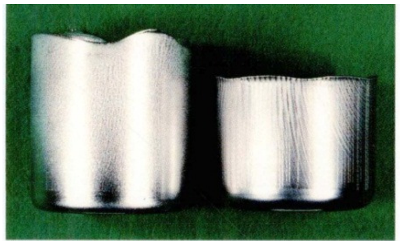


IF steel after rolling
A. Wauthier, PhD Paris 13, 2008



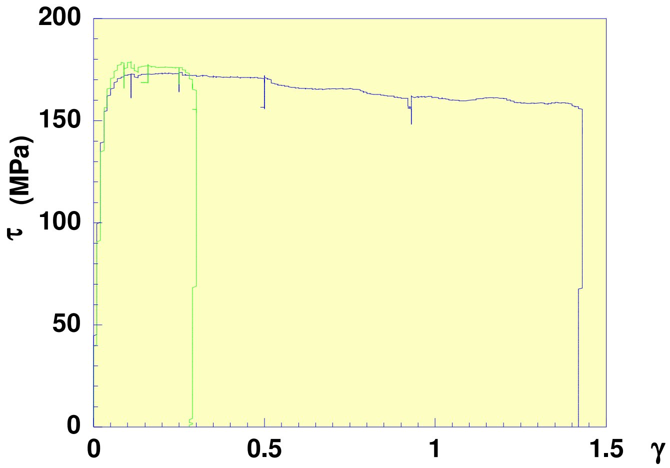
Zr alloy after recrystallization
K. Zhu, PhD Paris 13, 2006

Duplex steel after welding
R. Badji, PhD Paris 13, 2008



Introduction

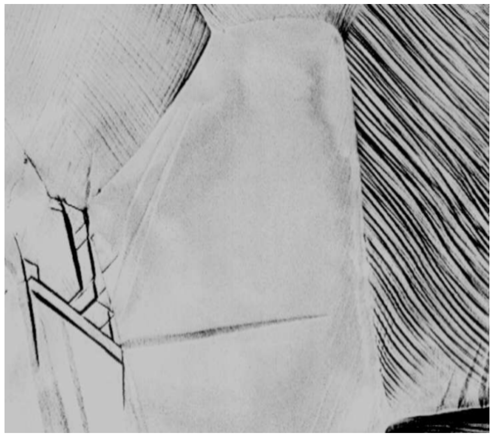
- Another example of macroscopic anisotropic behaviour



Al alloy (3004, hardened state) deformed in simple shear at 0° and 60° from RD. Same level stress but very different strains

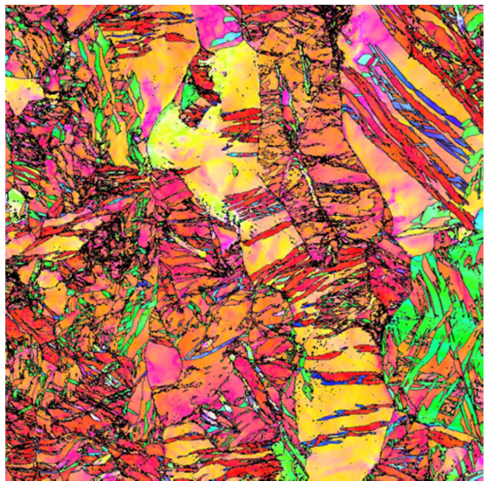
Gaspérini et al. J. Phys. IV France **11** (2001)

- We can also find some examples of « local » heterogeneities



Zr alloy deformed in uniaxial tension

Ti alloy deformed in plane strain compression

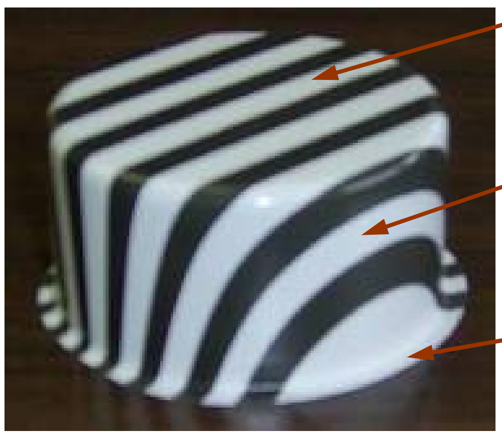


Aim of polycrystalline plasticity

To estimate the mechanical properties
To predict the texture evolution during forming
from the properties and repartition of the material constituants

Complex strain paths

Forming part for can making

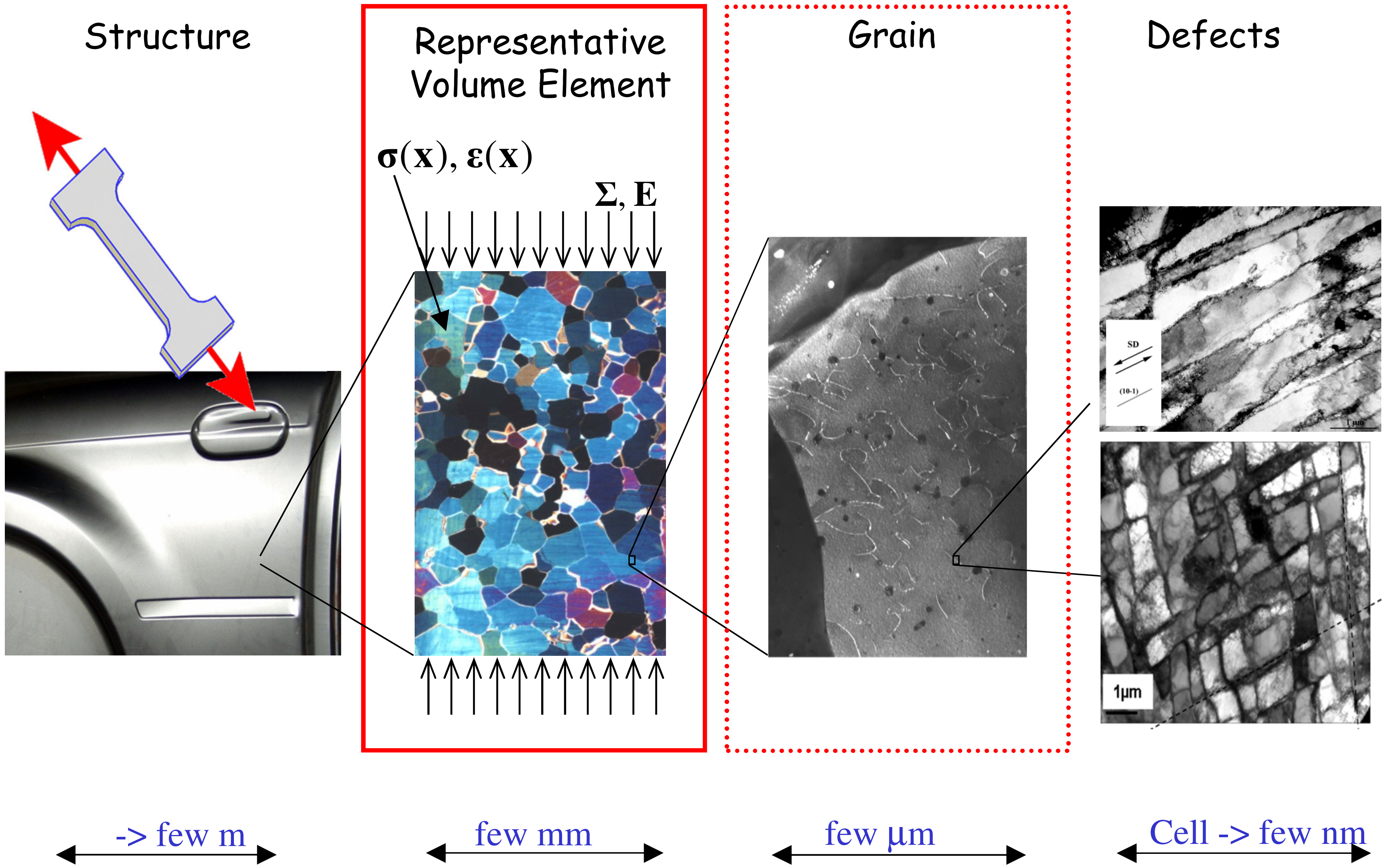


Steel for can making
C. Luis, PhD Paris 13, 2011

Outine

- The different scales of interest
- Experimental measurements and observations
- The different modelling approaches
- Some successfull examples
- Perspectives and open questions

At least 4 different scales which are of interest here



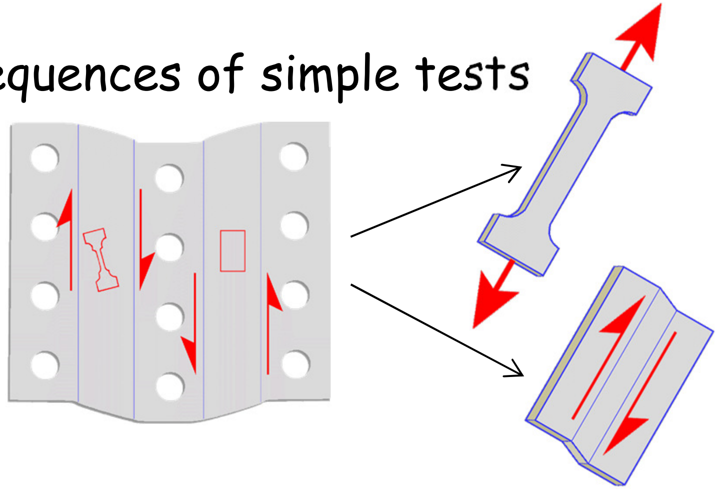
Outine

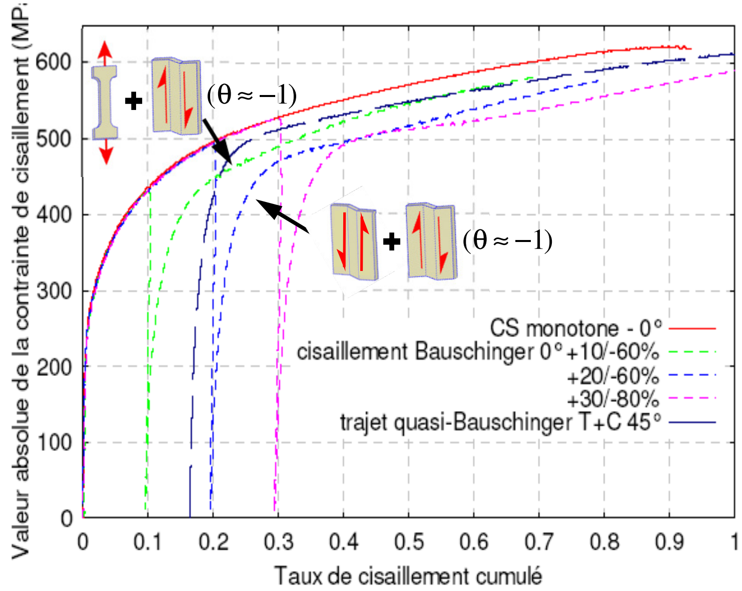
- The different scales of interest
- Experimental measurements and observations
- The different modelling approaches
- Some sucessfull examples
- Perspectives and open questions

Observations and measurements at various scales

At the level of the structure: the mechanical response: 3 main approaches

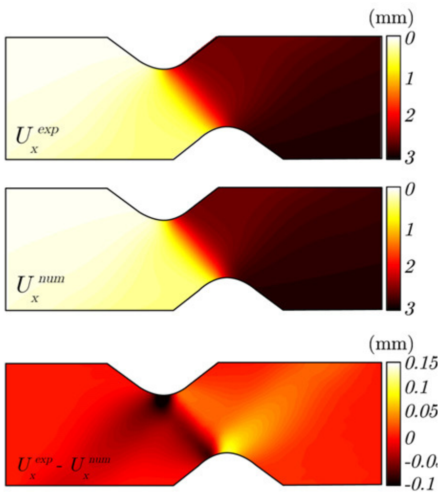
Sequences of simple tests



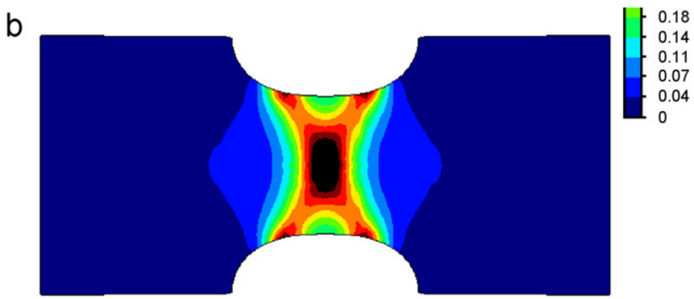


Bouvier et al. J Mater. Proc. Technol. 174 (2006)

One single heterogeneous test

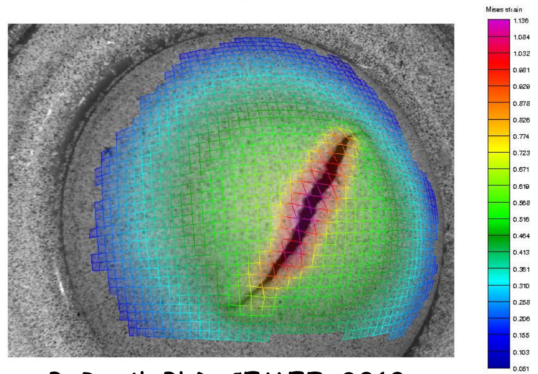


Pottier et al. Eur. J. Mech. 30 (2011)



Belhabib et a. Int. J. Mech. Sci. 50 (2008)

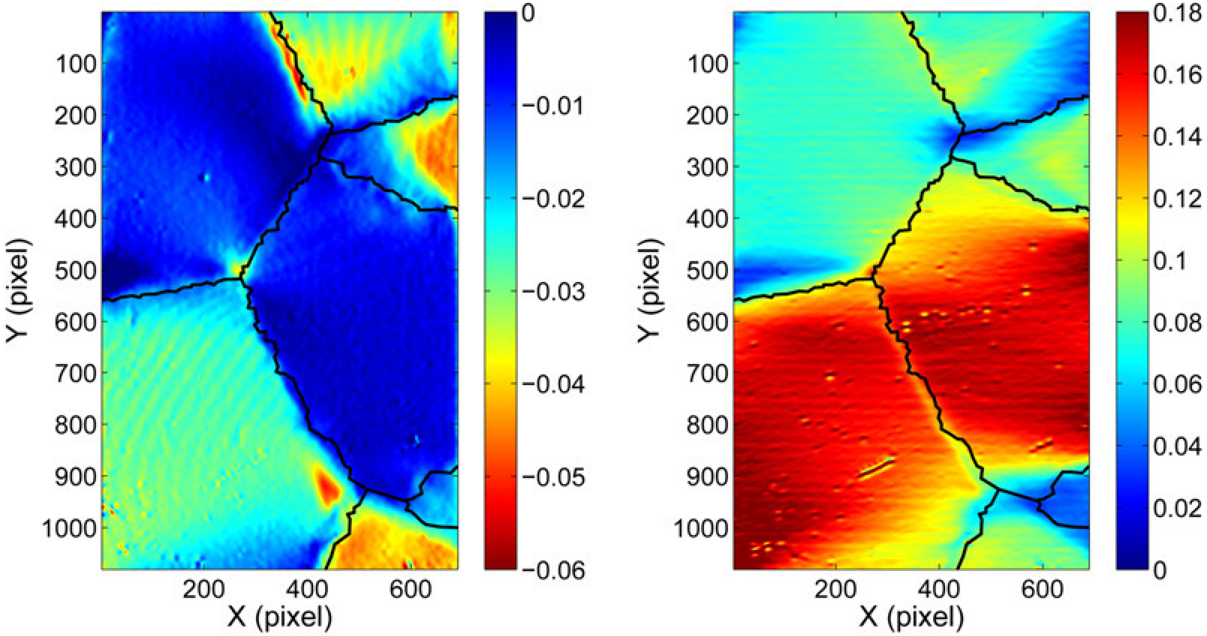
One forming operation



B. Revil, PhD CEMEF, 2010

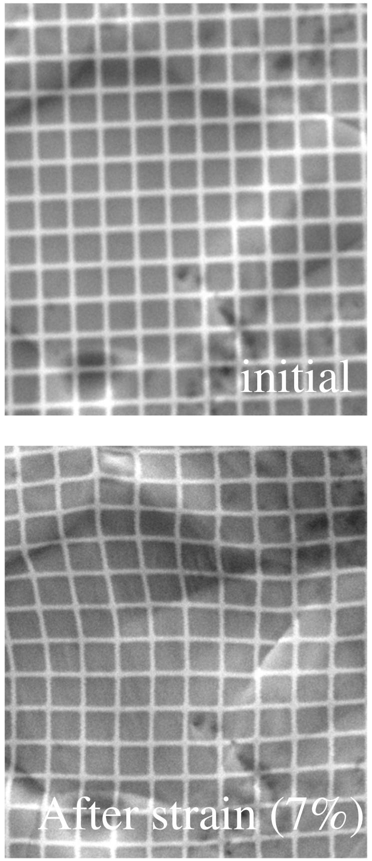
Observations and measurements at various scales

At the level of the RVE : orientation and displacement fields



a- E_{xx}, measurement   b- E_{yy}, measurement

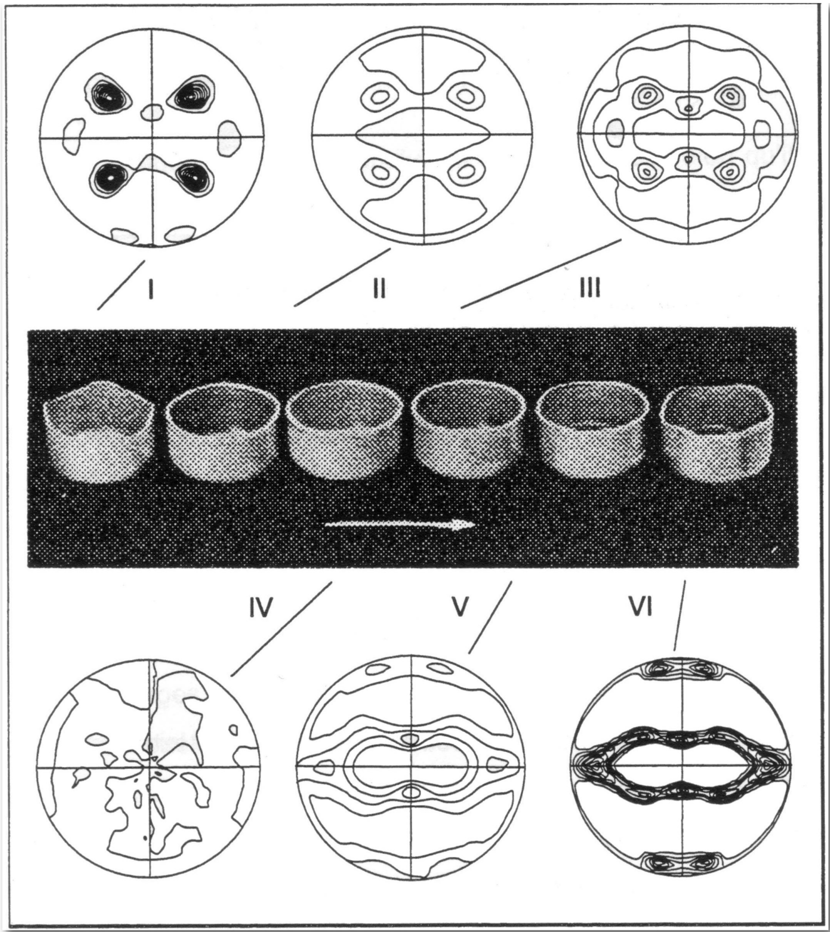
Al multicrystal deformed in tension – DIC technique
Badulescu et al., Mech. Mater. 43 (2011) 36–53



Zr alloy, grain size = 13 μm
M. Dexet, PhD, LMS, 2006

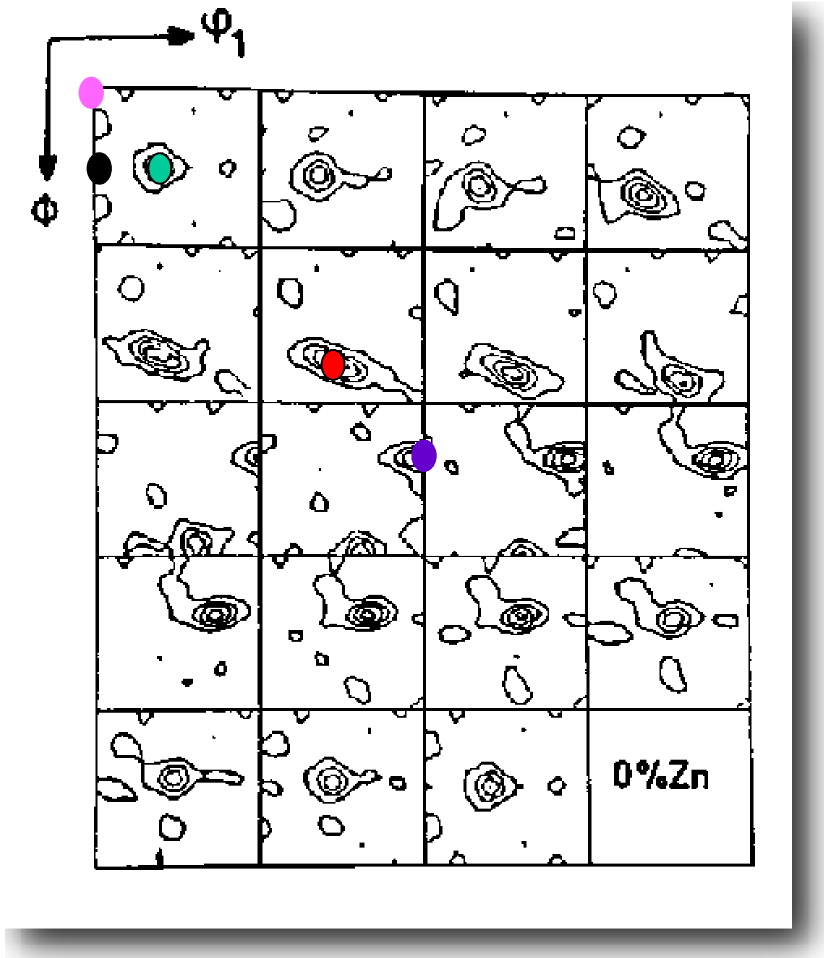
Observations and measurements at various scales

At the level of the RVE : crystallographic texture (pole figures and ODF)



Rodrigues, Bischel, Furrer (*1984*)

Bunge et Tobisch (*1968*), Virnich et Lücke (*1978*



Goss {110}<100>, Bs {110}<112>,
S {123}<634>, Cu {112}<111>, Cube {100}<001>

Observations and measurements at various scales

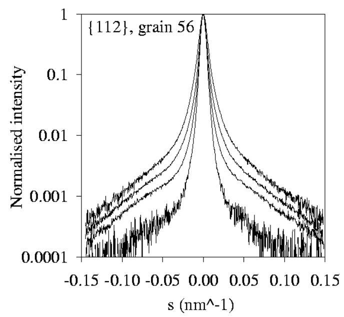
At the level of the grain and subgrain : orientation and morphology (EBSD), dislocation density and /or stored energy

From XRD, EBSD, TEM
Also Disclination density from EBSD (Beausir & Fressengeas 2012)

Average cut-off radius

$$E_g = \alpha \mu b^2 \rho_g \ln \frac{R_e}{b}$$

Average density



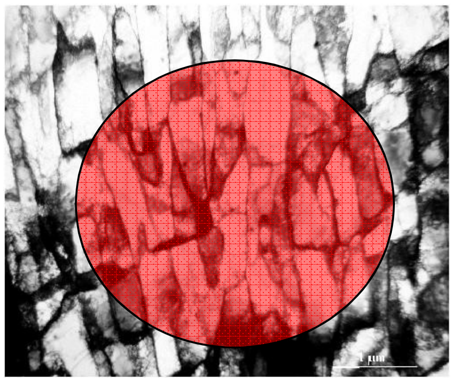
$$\ln|A(n)| = -\frac{\pi}{2} K^2 b^2 n^2 C \rho_g \ln\left(\frac{R_e}{n}\right) + o(n)$$

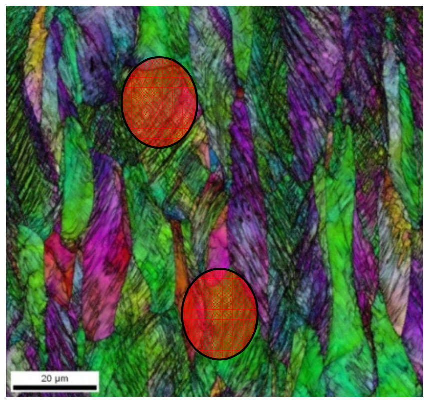
K = diffraction vector mudulus
C = contrast factor of dislocations

Average misorientation

$$E_{wg} = \frac{2}{\delta_g} \gamma_m \frac{\theta_g}{\theta_m}\left(1 - \ln \frac{\theta_g}{\theta_m}\right)$$

Average cell size

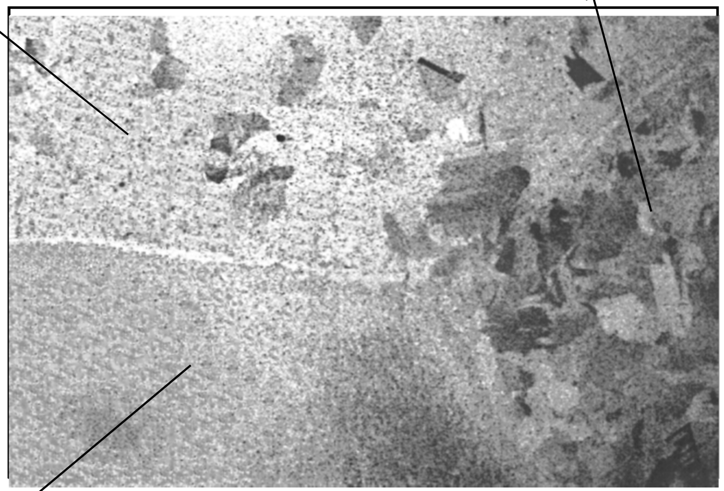




Observations and measurements at various scales

Partial REX
E_2 = 15.1 J/mol.

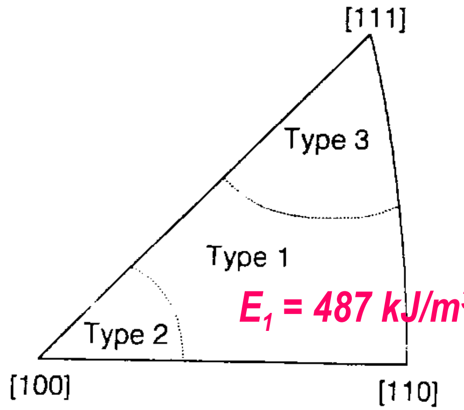
Complete REX
E_1 = 17.3 J/mol.



No REX
E_3 = 11.8 J/mol.

In situ recrystallisation
Cu multicrystal after rolling
Mohamed and Bacroix, 2000

E_3 = 749 kJ/m^3 (3.6, 1.5)



E_1 = 487 kJ/m^3 (2.1, 1.2)

E_2 = 363 kJ/m^3 (1.7, 0.8)

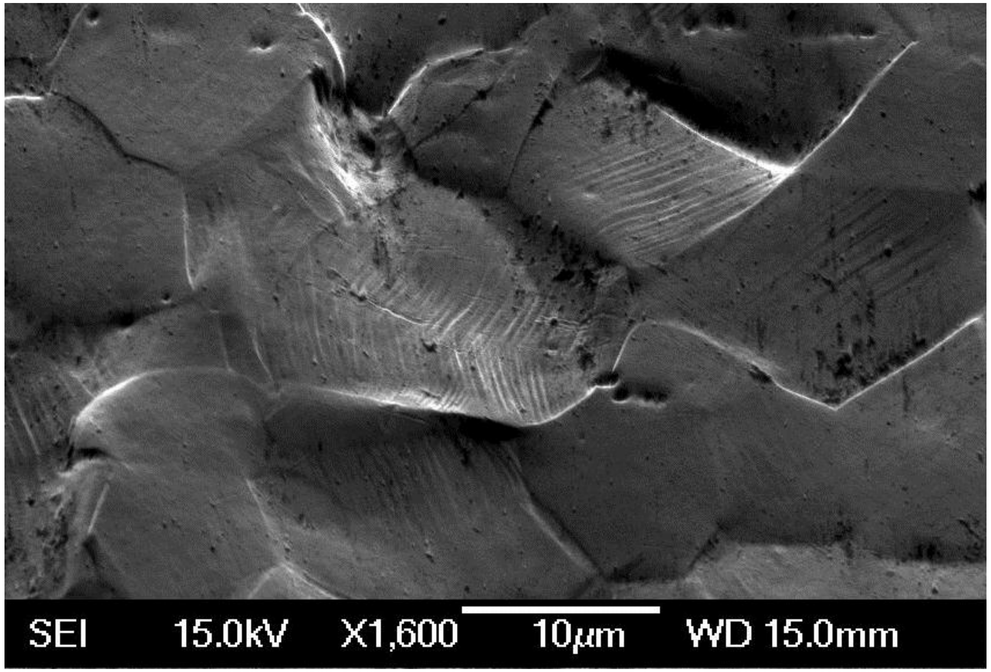
SIBM of <100> grain into <111> grains
after tension in Cu (e=0.3)
(Huang et al. 1999)

Strong link between SE and
recrystallization mechanisms

Cu, cold drawn (40%)
E<100> = 1.8 and E<111> = 3.6 J/mol.
Neutron Diffraction
Samet-Meziou et al., Mat. Sci. Eng. A 528 (2011)

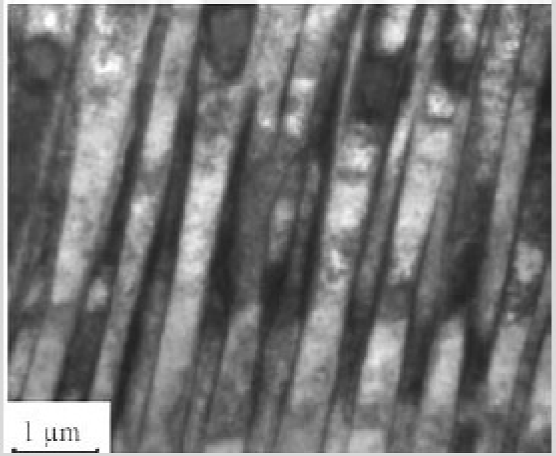
On-going Comparative investigation of various
measurement types in GDR Rex 3436
« Recrystallization and Grain Growth », (R. Logé)

Observations and measurements at various scales



FEG-SEM
Pure Ti rolled 30%:
Prism <a> activity goes from 50 to 25%
Pyr<c+a> activity goes from 0 to 40%
A Chattopadhyay et al.. *Materials Science and Technology*, 2011

Bright field images

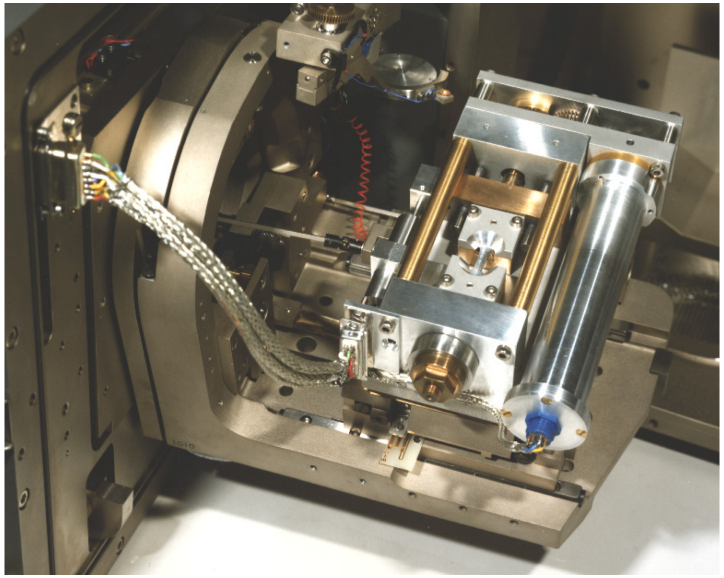


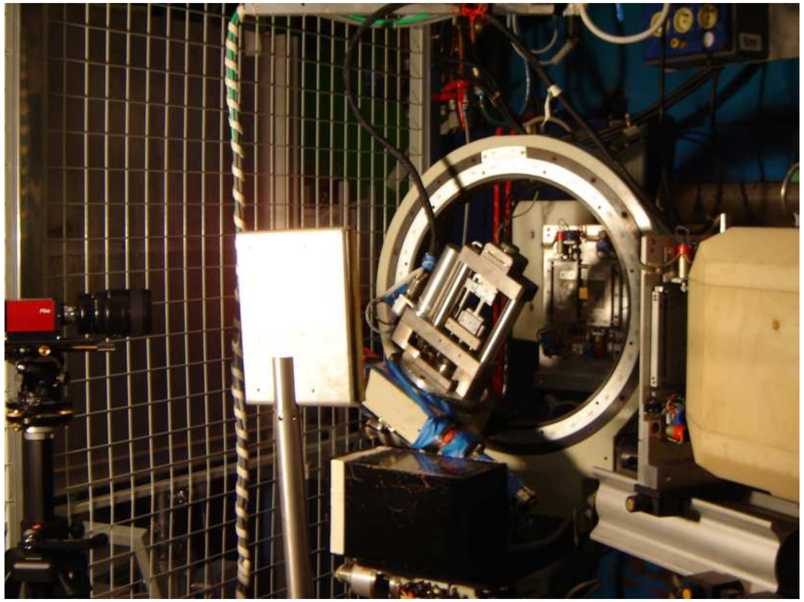
Deformed steel

Orientation maps

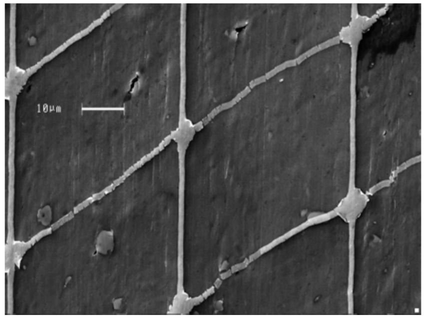
ASTAR, SIMAP

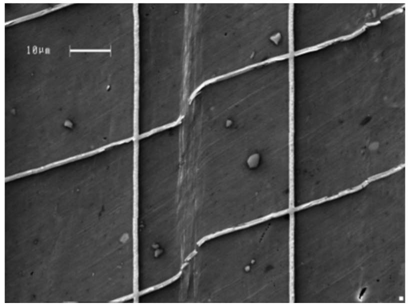
Observations and measurements at various scales

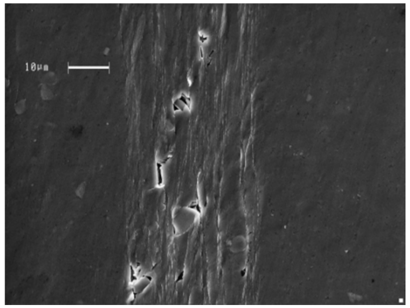




Micro-machines for in situ investigations
SEM – LSPM (left), LLB(right)







Gaspérini et al. J. Phys. IV France **11** (2001)

5182 alloy, deformed in simple shear (0 and 60°/RD)

Sharp shear-banding: Damaging effect of particles

Outine

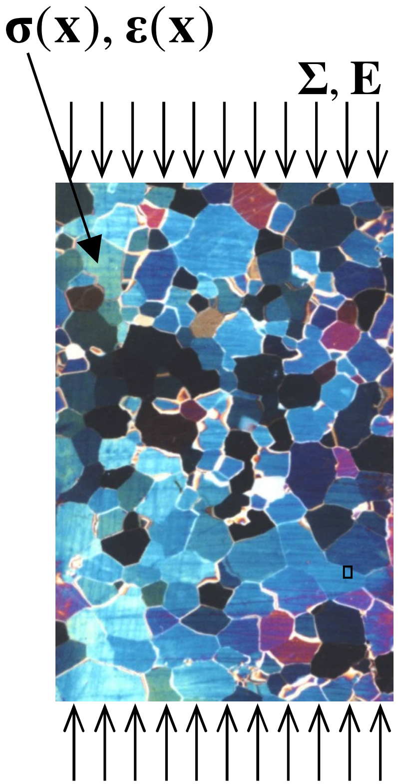
- The different scales of interest
- Experimental measurements and observations

  Macroscopic curves, textures, strain fields, slip mechanisms, dislocation density

- The different modeling approaches

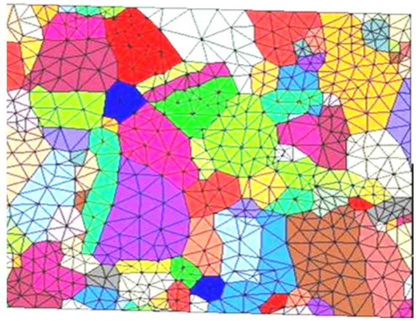
- Some successful examples
- Perspectives and open questions

Micro-mechanical modelling: 2 main approaches



Full Field Approaches (FEM, FFT, …)

☹ → needs powerful computers
→ good precision even for non-linear behaviours
→ full stress and strain fields
☹ → but full fields are still rarely necessary
☹ → up to now, the real microstructure is over-simplified

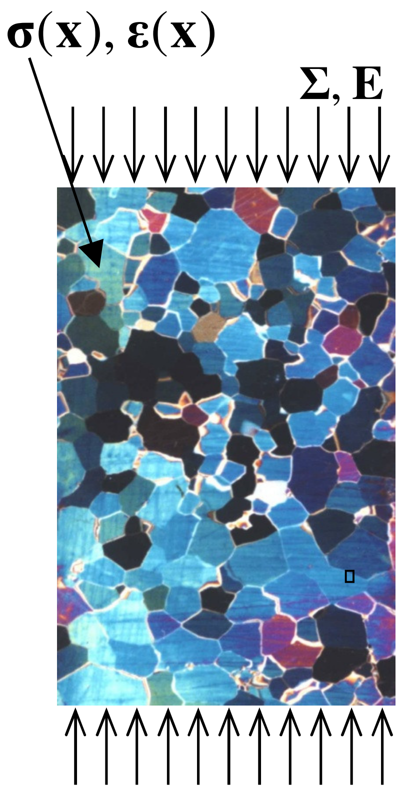


Mean field approaches (e.g. SC model)

→ an exact solution for some specific microstructures and behaviours
→ furnishes bounds
→ rapid calculations to get a statistical information
→ but non – linearity not obvious to treat
→ microstructure evolution less precise

Microstructure described statistically

Micro-mechanical modelling: recent developments



Full Field Approaches (FEM, FFT, …)

CPFE Pierce et al. 1982
Crystalline UMAT in Abaqus (Huang 1991)
Numerical mesoscope, S. Héraud, PhD, 1998, Dexet 2006
Crystalline EF, Cailletaud, Forest & coworkers (from 2000)
FFT Lebensohn, Tomé, Ponte Castañeda (2007)
A. Belkhabazz, PhD 2012, ...

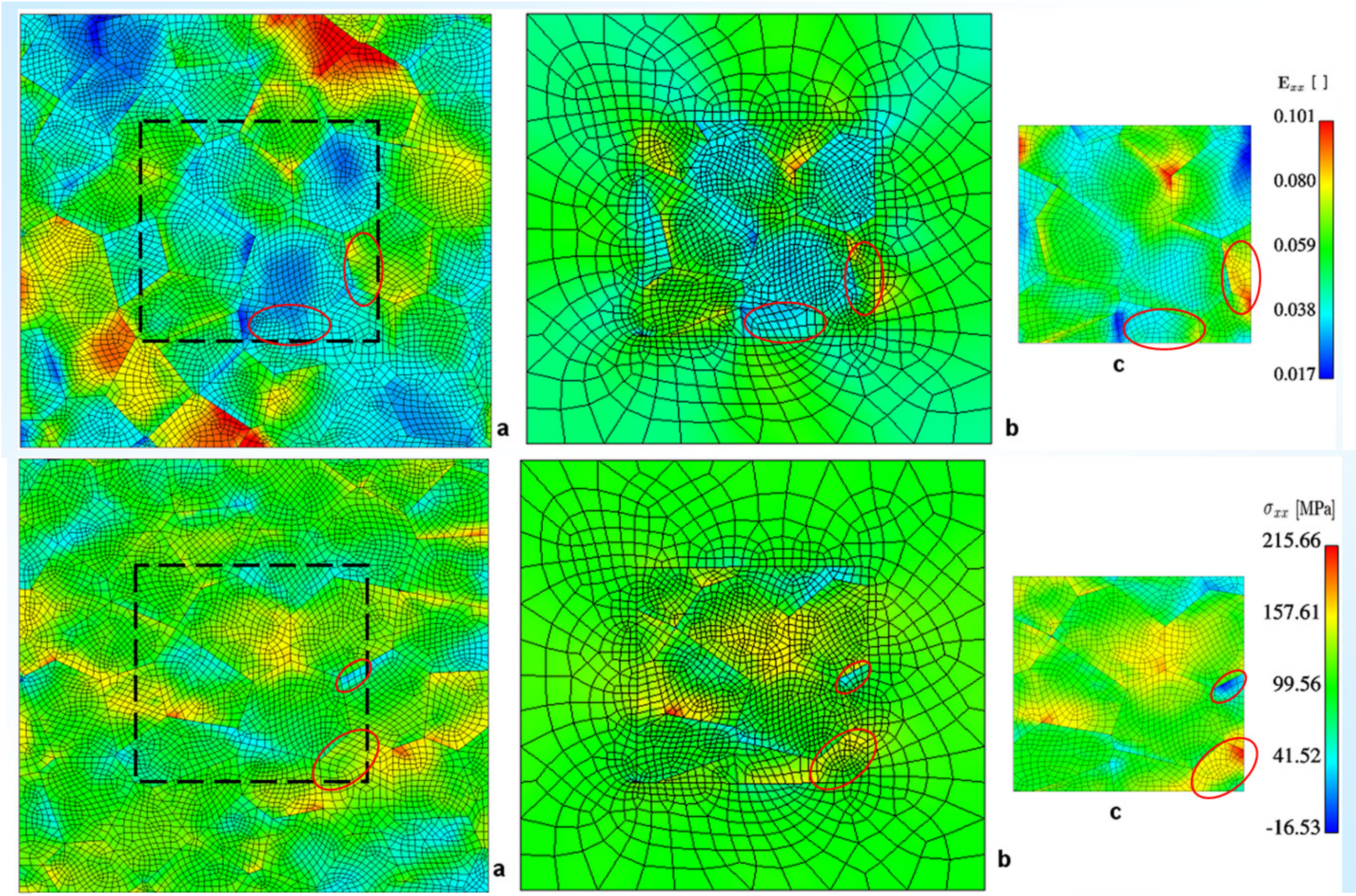
Mean field approaches

. 1928 : Sachs, proportional stress
. 1938 : Taylor, uniform strain – Upper bound
(s = 3.06 t_0, tension, isotropic fcc)
. 1965 : Hill, incremental
. 1979 : Berveiller et Zaoui, secant
. 1987 : Molinari, Canova et Ahzi, tangent
. 1991 : Ponte Castaneda, variational – upper bound
. 1995 : Suquet, modified secant
. 1996 : Ponte Castaneda, second order
. 1999 : Masson et Zaoui, affine
Talbot et Willis (1985), Lebensohn &Tomé (1993), ….

Few examples of full field calculations

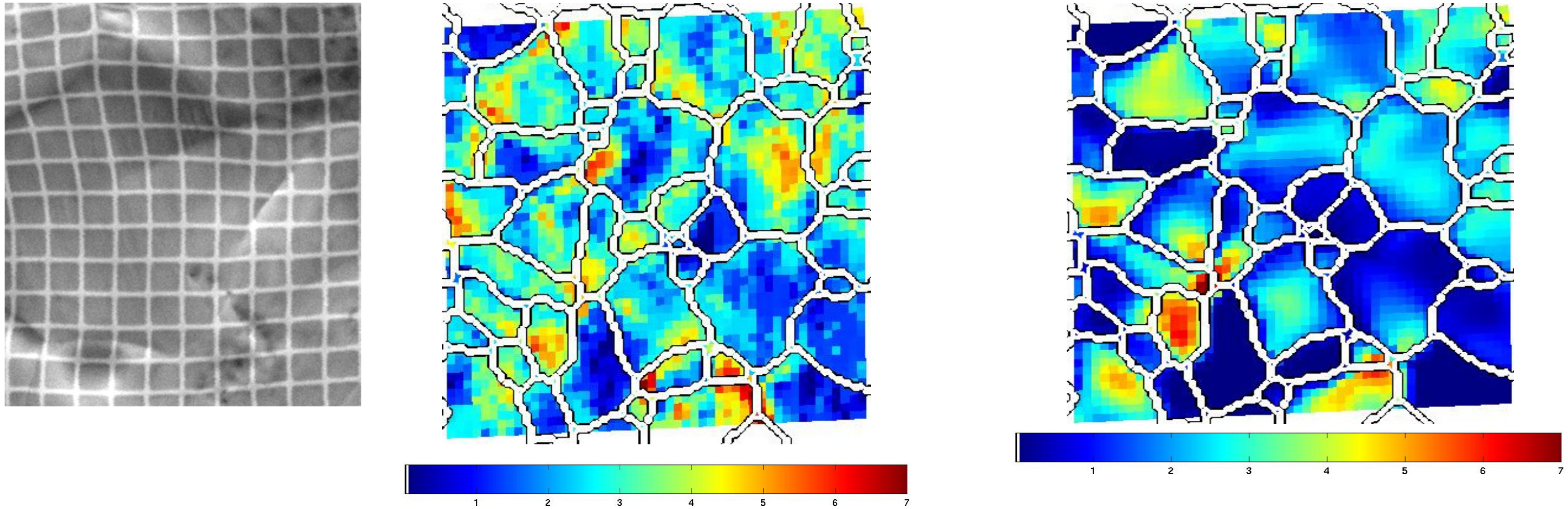
Numerical mesoscope, Meso3D

[Haddadi and Salahouelhadj, 2005]



(a) reference plate (b) mesoscope (c) motif alone

Few examples of full field calculations



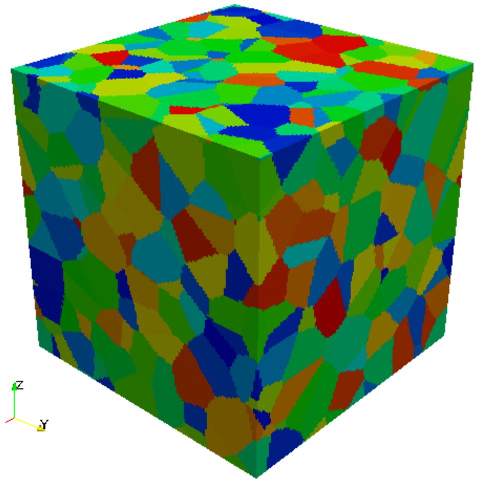
Polycrystalline Zr,
FE simulations with mesoscope, M. Dexet, 2006
Experimental and simulated axial strain (7%)

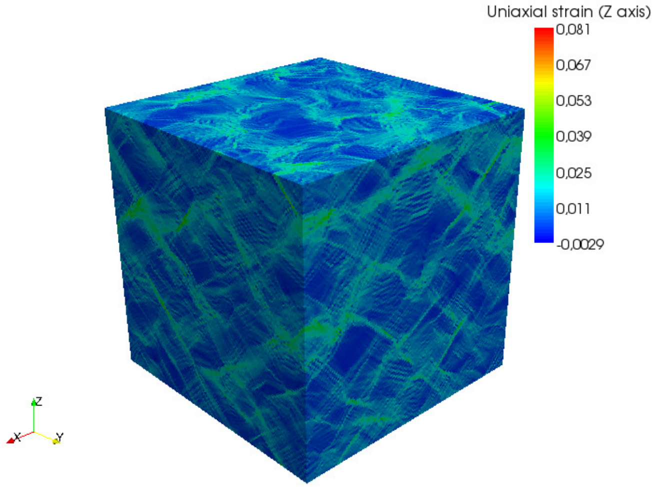
The simulation is also used to identify the hardening law

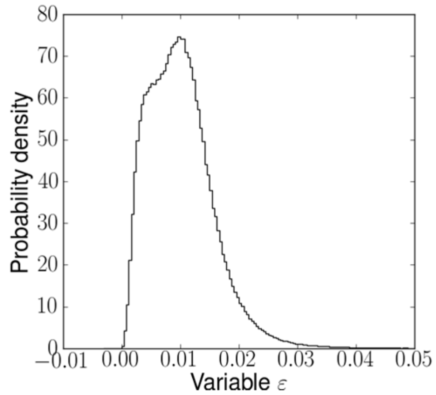
Few examples of full field calculations

Elasto-plastic behaviour of fcc polycrystals in tension by FFT

Axial strain field





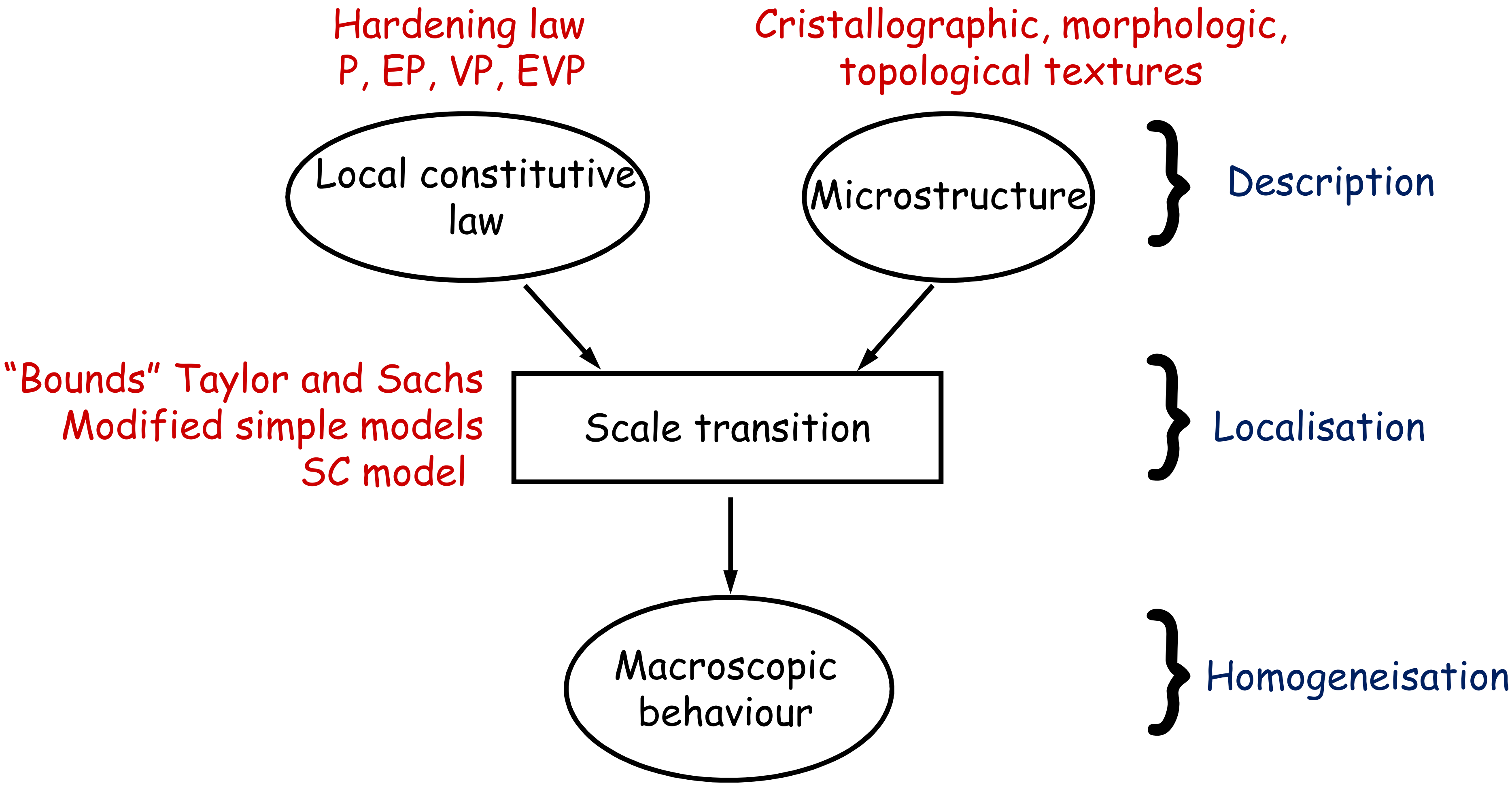


✔ Deformation bans at 45°consistent with experimental observations (Doumalin, 2000 – Moulart et al. , 2009 …)

✔ Strong asymétrie of the strain field distribution

R. Brenner, 2010

The mean field approach, applied to the polycrystals



Output : Macroscopic behaviour

+

Texture evolution + Mechanical Properties + Active systems

The mean field approach, applied to polycrystals

The microscopic hardening law

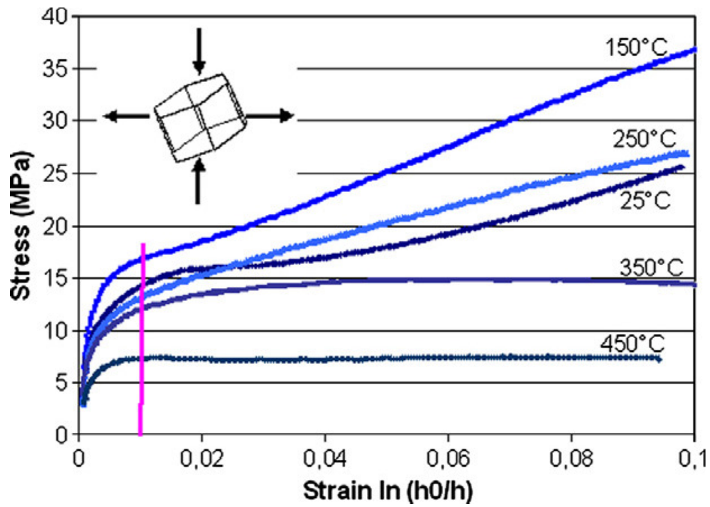
Saturating hardening law

$$\dot{\tau}_0^{(s)} = \sum_l h^{sl} \left|\dot{\gamma}^{(s)}\right| \qquad h^{sl} = q^{sl}\left(1 - \frac{\tau_0^l}{\tau_{sat}}\right)^a$$

Dislocation – based hardening law

$$\tau_0^{(s)} = \alpha\mu b \sqrt{\sum_l h^{sl}\rho^l}$$

$$\dot{\rho}^{(s)} = \frac{1}{b}\left(\frac{\sqrt{\sum_l a^{sl}\rho^l}}{K} - 2y_c\rho^{(s)}\right)$$



Mg single crystals, Chapuis & Driver 2011

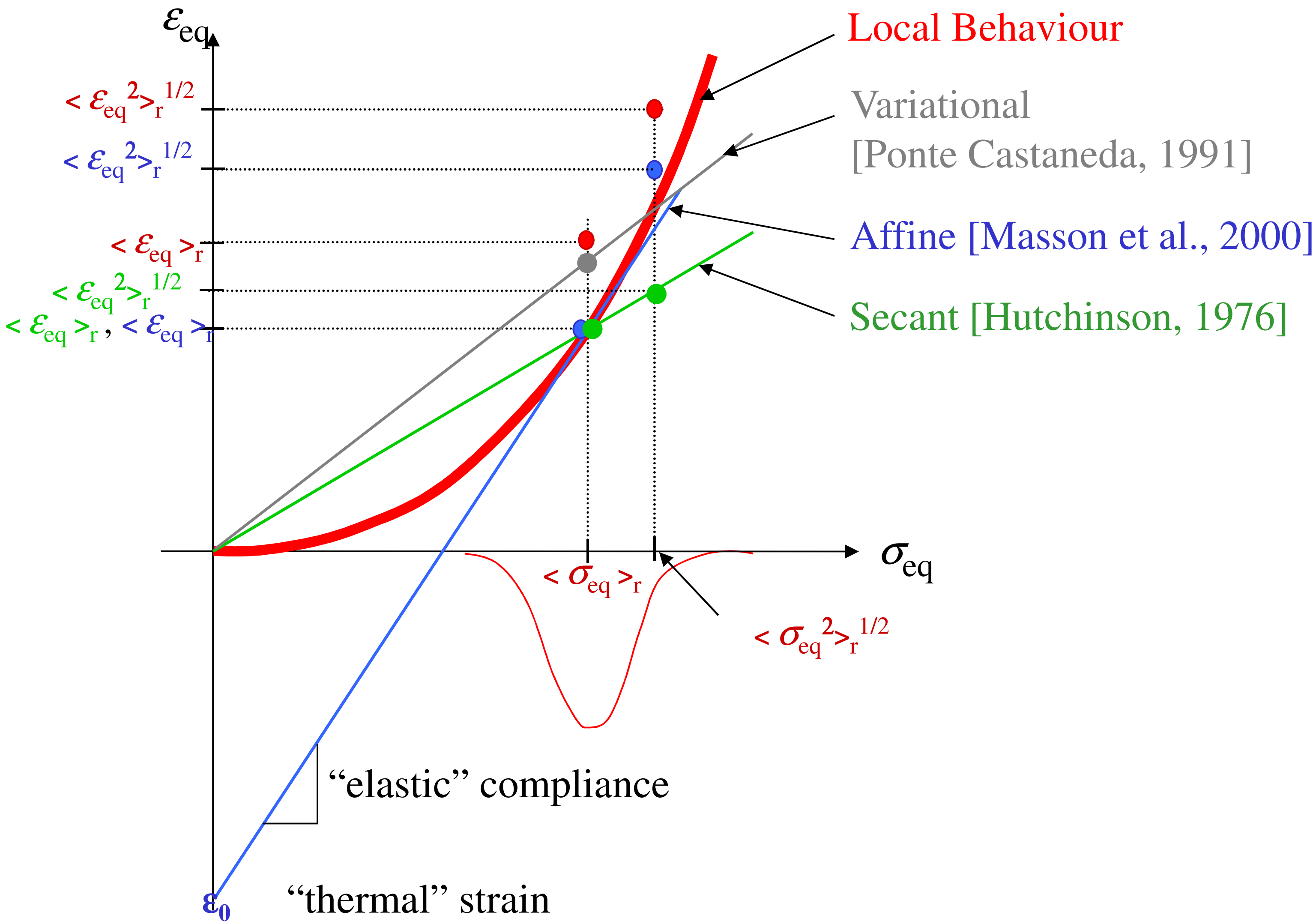
Interactions coefficients ≠ for coplanar, colinear, orthogonal slip
Possibility of adding other contributions
(kinematic hardening, size effect)

The mean field approach, applied to polycrystals

Localisation step (P, EP, VP, EVP)

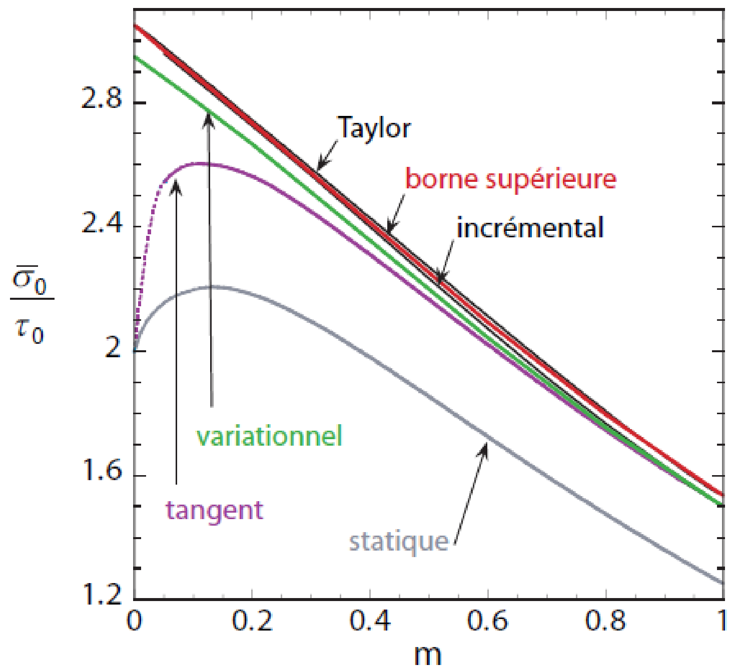
In thermoelasticity $\boldsymbol{\varepsilon}(\mathbf{x}) = \mathbf{s}(\mathbf{x}) : \boldsymbol{\sigma}(\mathbf{x}) + \boldsymbol{\varepsilon}^0(\mathbf{x}) \longrightarrow \boldsymbol{\sigma}(\mathbf{x}) = \mathbf{B}(\mathbf{x}) : \overline{\boldsymbol{\sigma}} + \boldsymbol{\sigma}_{res}(\mathbf{x})$

In viscoplasticity $\boldsymbol{d}^g = \boldsymbol{M}^g : \boldsymbol{\sigma}^g + \boldsymbol{d}_0^g, \quad \boldsymbol{D} = \overline{\boldsymbol{M}} : \boldsymbol{\Sigma} + \boldsymbol{D}_0,$



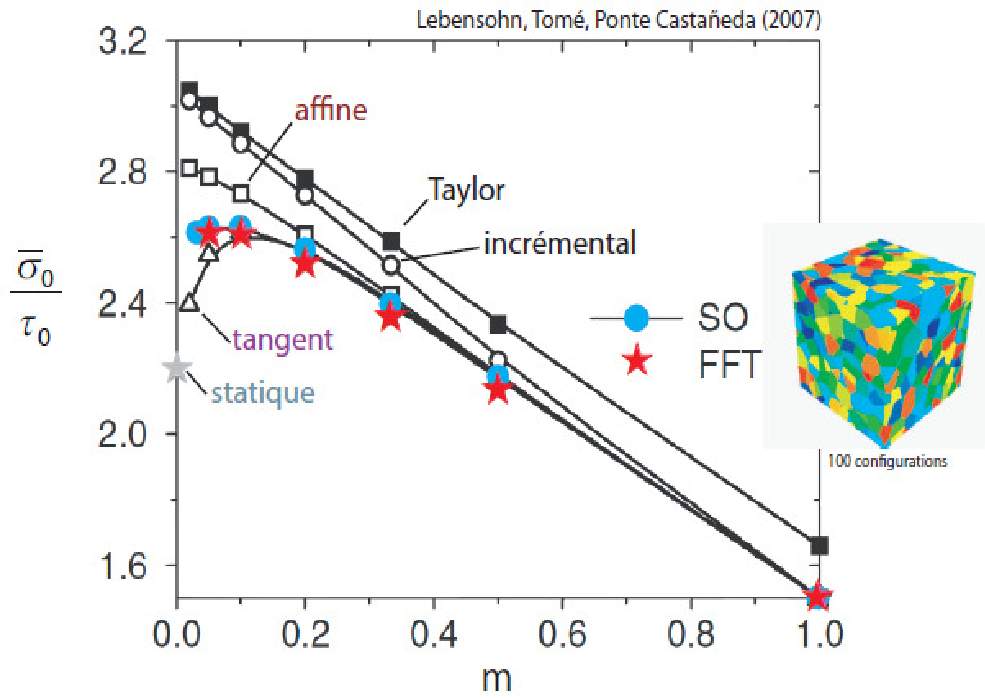
The mean field approach, applied to polycrystals

Comparison of models in viscoplasticity: isotropic fcc polycristal



Mean field

Full field



P. Gilormini, EC2M, 2010

Outine

- The different scales of interest
- Experimental measurements and observations

  Macroscopic curves, textures, strain fields,

  slip mechanisms, dislocation density
- The different modeling approaches

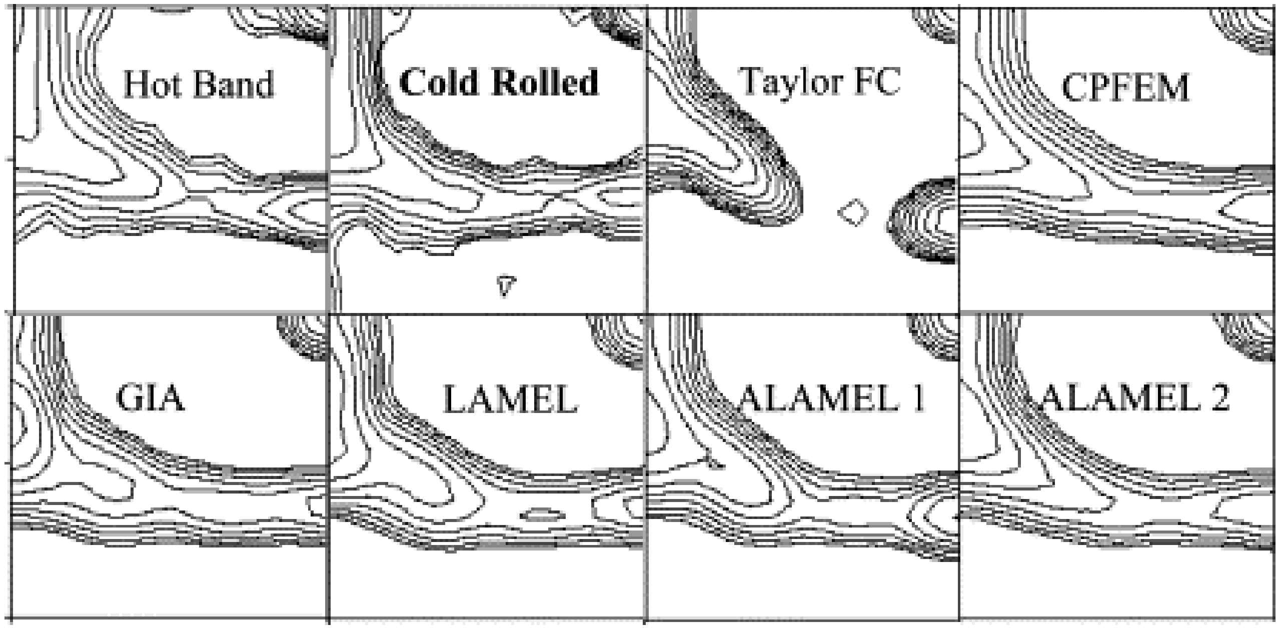
- Some successful examples

- Perspectives and open questions

The mean field approach, applied to polycrystals

Identification – Validation: how to proceed ?

Identification on one single curve and validation on textures

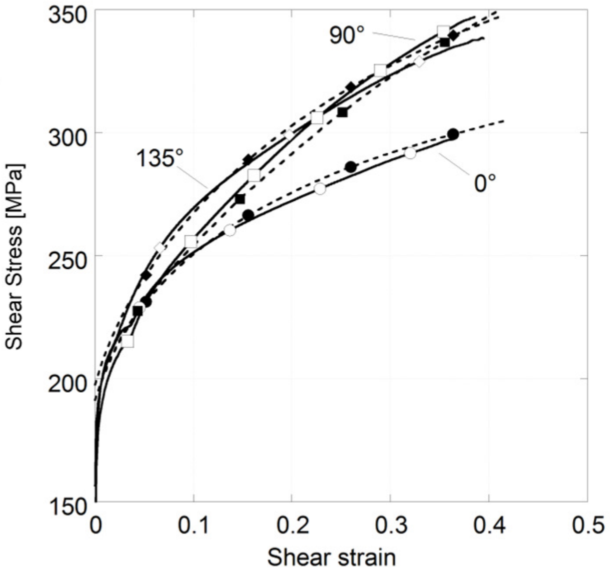


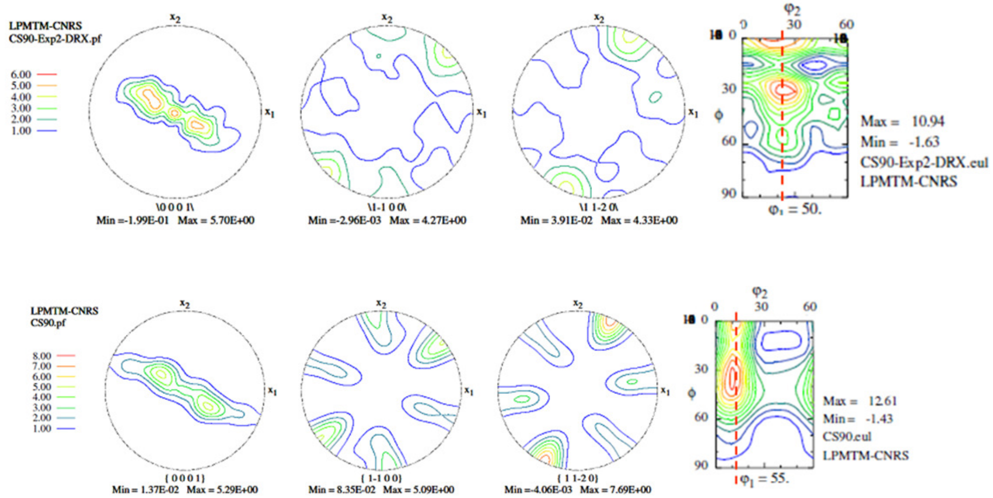
LAMEL Models better; OK but the slip systems are known and the identification is made on one single model !!!

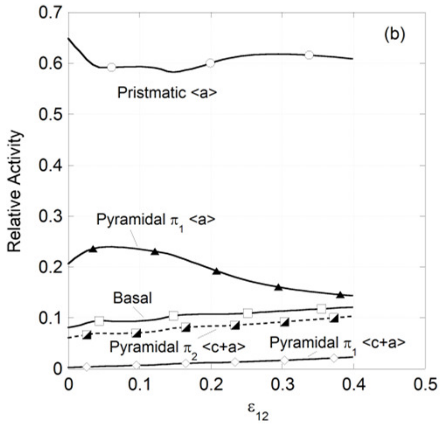
Van Houtte et al, 2008

The mean field approach, applied to polycrystals

Case of Ti (Benmhenni 2012, PhD Paris 13), identification on 3 curves, validation on textures and R(α), verification on activity of systems



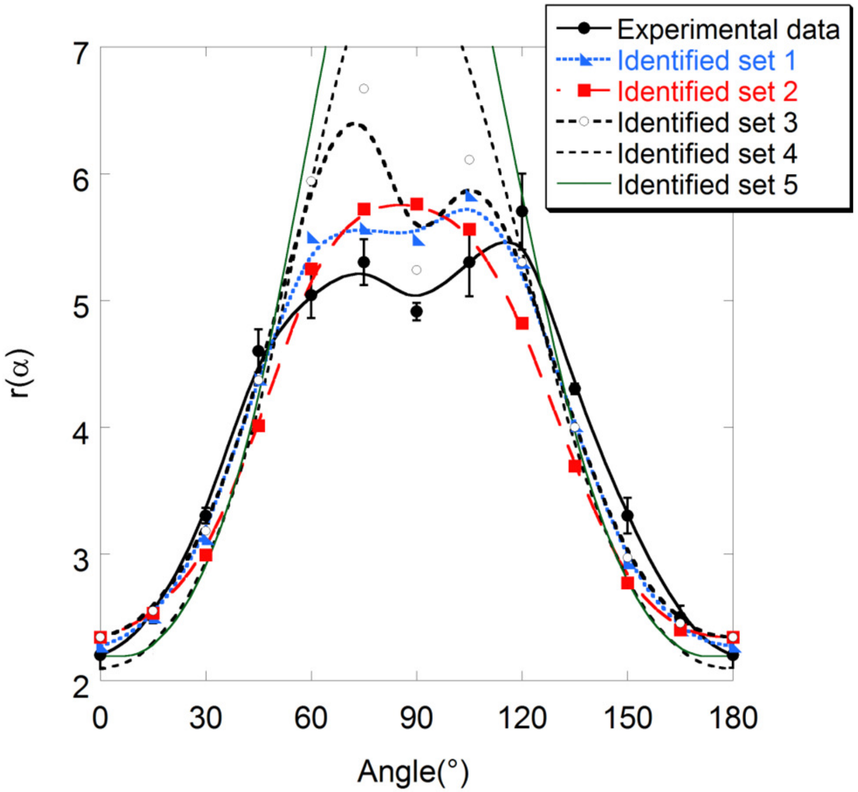


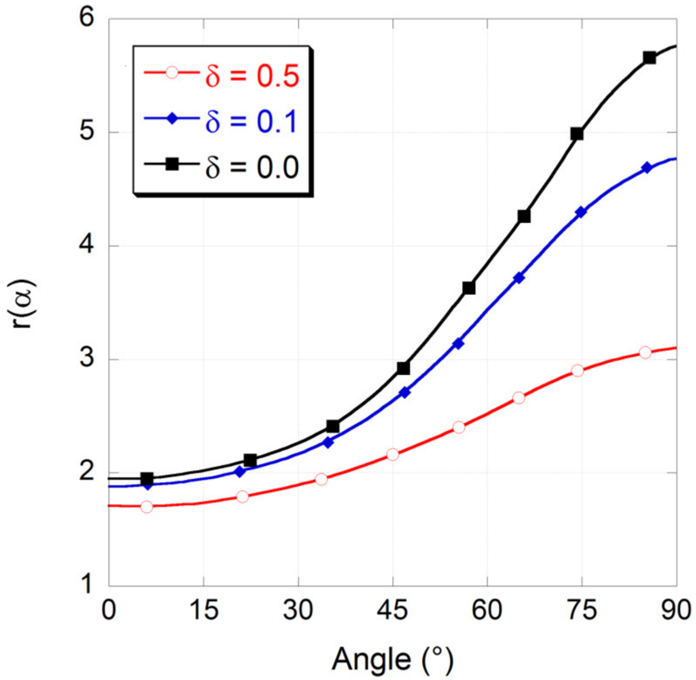


Activities of systems consistent
With experimental observations
(LEM3, Metz)

The mean field approach, applied to polycrystals

Case of Ti (Benmhenni 2012), identification on 3 curves, validation on textures and R(α), verification on activity of systems

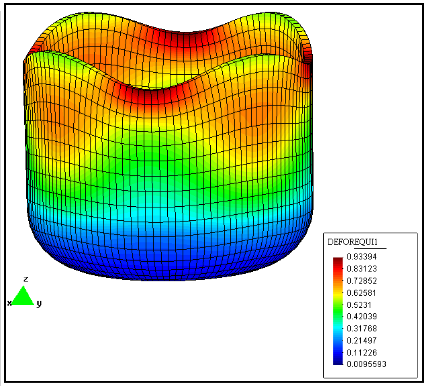


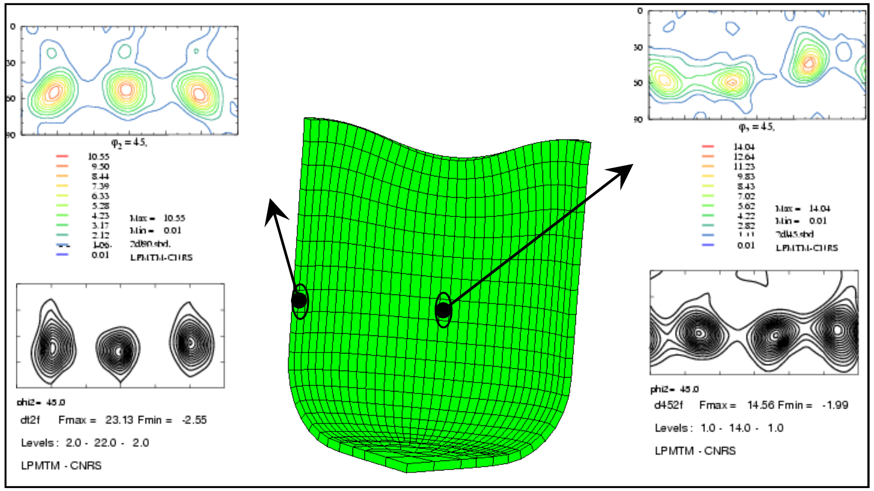


Pb: strong sensitivity of R to the texture spread

The mean field approach used to identify a plastic potential for FE simulations of a structure

- *ABAQUS simulation*
- *IF Steel*
- *Plastic potential identified on texture*
- *Isotropic hardening law identified on simple tests*





S. Bouvier et al.

Outine

- The different scales of interest
- Experimental measurements and observations
- The different modelling approaches
- Some successful examples

- Open questions and perspectives

The mean field approach, applied to polycrystals

Some cases are less good:

- Simulations with twinning (several approches)
- Large deformations
- Strong anisotropy at the level of the crystal (olivine)

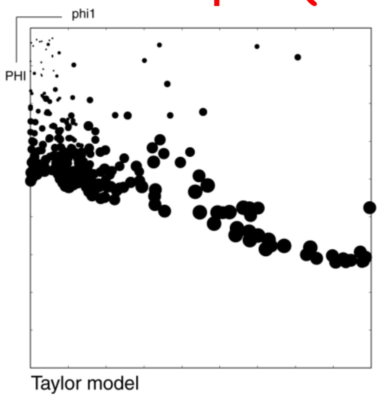
One missing ingredient : fragmentation of grains due to dislocations (Toth, Bouaziz, Peeters et al. 2001, …..); localization of strain

Old idea already present in Taylor RC, Lamel, Arminjon, ……

Some remaining difficulties

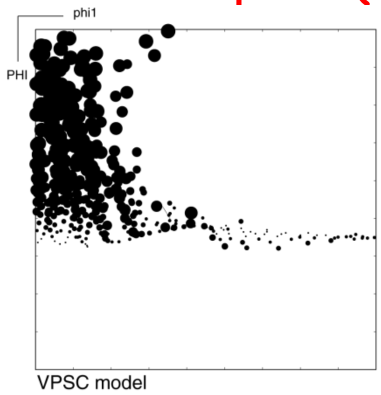
The calculated SE depends strongly on the selected model: ex. of steel

Simple (Taylor)



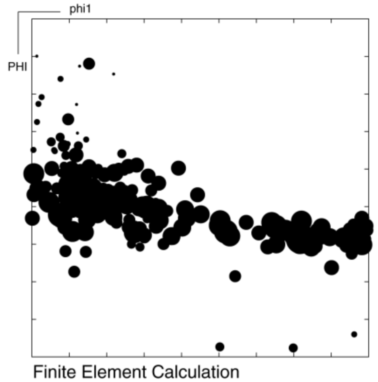
Hard grains = γ fiber
Oriented Nucleation

Complex (SC)



Hard grains = α fiber
SIBM

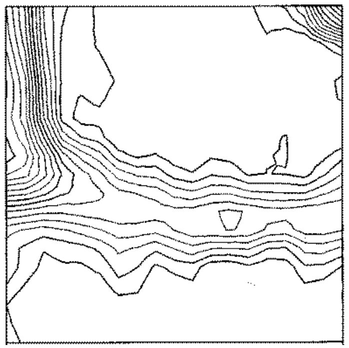
FEM

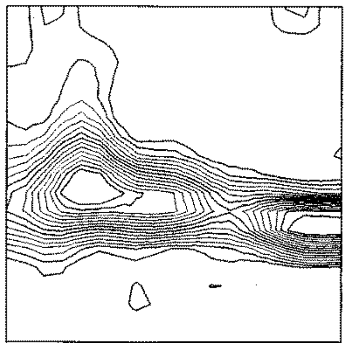


Hard grains = γ fiber

Bacroix et al., Modelling Simul. Mater. Sci. Eng., 7(1999).

Exp. Rolling

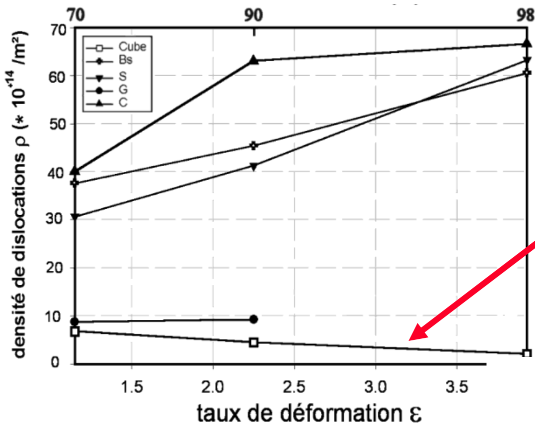




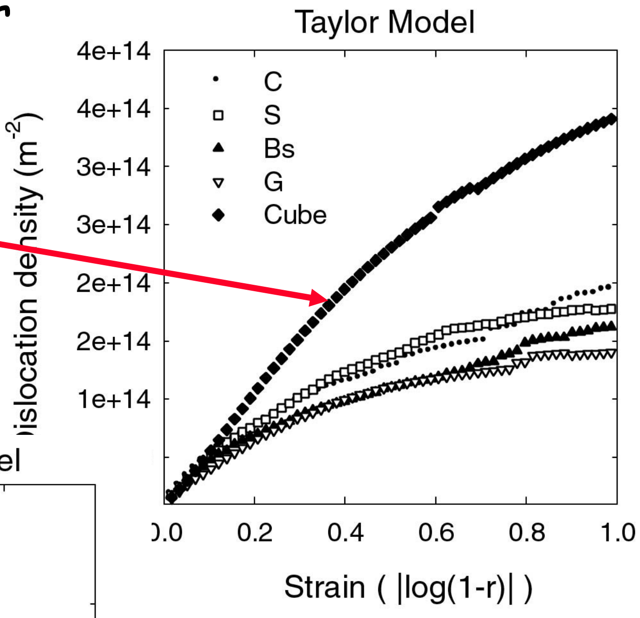
Exp. Annealing

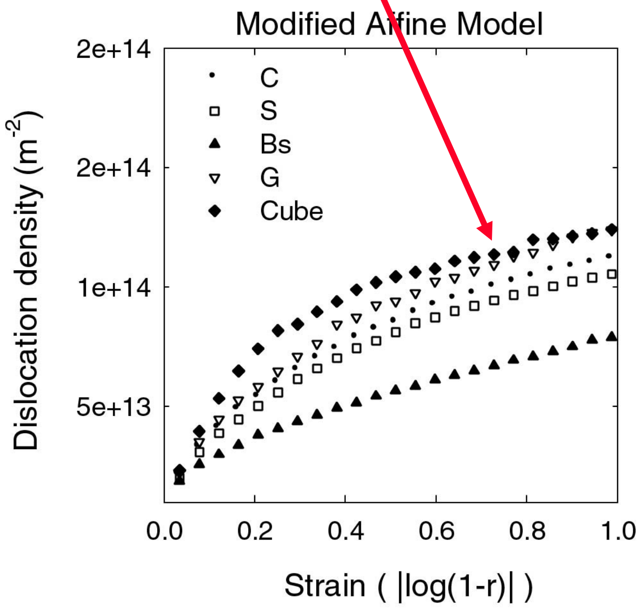
Some remaining difficulties

Hardening within specific orientations in copper



Orientation Cube





Strong recovery observed but strong hardening predicited

A proposed indirect recovery mechanism

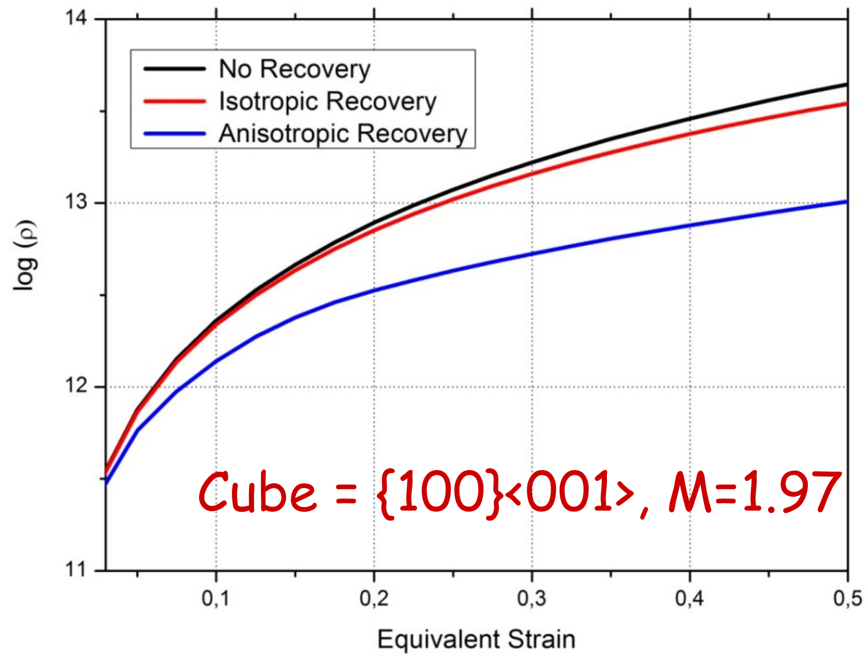
$$\tau_0^{(s)} = \alpha\mu b\sqrt{\sum_l h^{sl}\rho^l} \quad \text{and} \quad \dot{\rho}^{(s)} = \frac{1}{b}\left(\frac{\sqrt{\sum_l a^{sl}\rho^{(l)}}}{K} - 2\sum_l b^{sl}\rho^{(l)}\right)$$

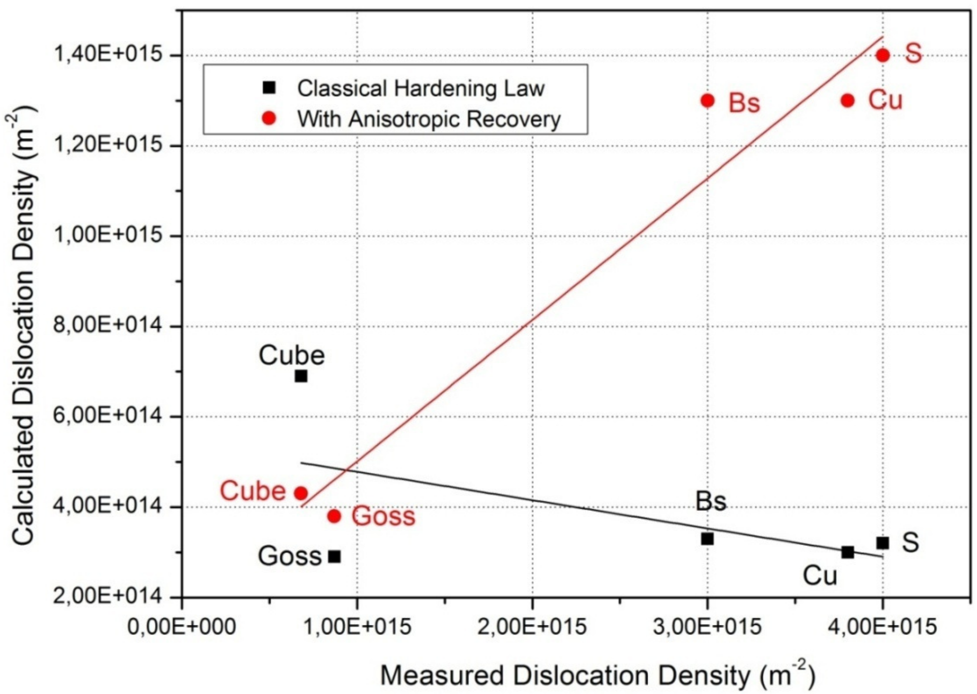
Possible interactions parameters:
self, coplanar, colinear, orthogonal, other

Hardening: 5 ≠ parameters
Recovery: 2 ≠ parameters only (orthogonal and non-orthogonal)

Taken from litterature
Tabourot et al. (identification), Kubin et al. (DDD)
Main difference: strong colinear interaction predicted from DDD

A proposed indirect recovery mechanism





Principal textures components in rolled copper

Bacroix & Brenner, Comp. Mat. Sci. 54(2012

Conclusions and perspectives

- Micromechanical approach useful for the understanding of the physical mechanisms, but not totally predictive yet
- Need to develop the full field approaches and a more and more precise and complete comparison with experimental data
- More work on single crystals (know – how is disappearing)
- In situ complex strain paths and field measurements
- Coupling of models (deformation and recrystallisation), of phenomena (plasticity and transformation, …..), of properties (magneto – mechanic coupling) ….

Two important books

U. F. Kocks, C. N. Tomé, H. -R. Wenk
Texture and Anisotropy: Preferred Orientations in Polycrystals and their Effect on Materials Properties
Cambridge University Press, 2000

Homogénéisation en mécanique des matériaux 1&2
(Traité MIM, série alliages métalliques)
Sous la direction de M. Bornert, Th., Bretheau et P. Gilormini (2001)