

# Couplages thermomécaniques durant la déformation plastique de polycristaux métalliques

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# Outline

## 1 Motivations

## 2 Experiment and data treatments

## 3 Results and analysis

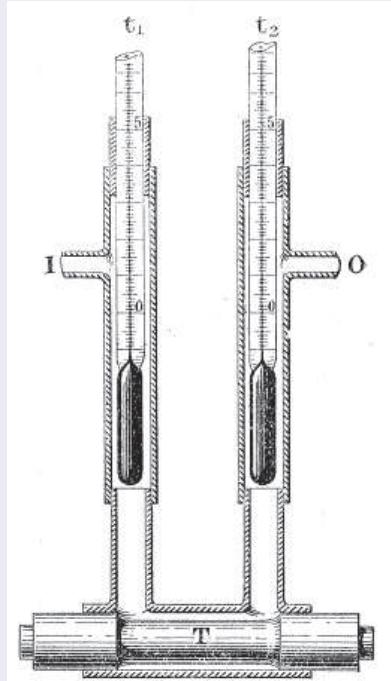
- Multi-scale yield stress identification
- Energy balance within polycrystals

## 4 Conclusions and prospects

## Self-heating tests

*The Determination of Fatigue Limits under Alternating Stress Conditions.*

By C. E. STROMEYER.

(Communicated by Prof. W. E. Dalby, F.R.S. Received March 26,—  
Read May 21, 1914.)

[Stromeyer, Proc. Roy. Soc., 1914]

## Fatigue limit and temperature

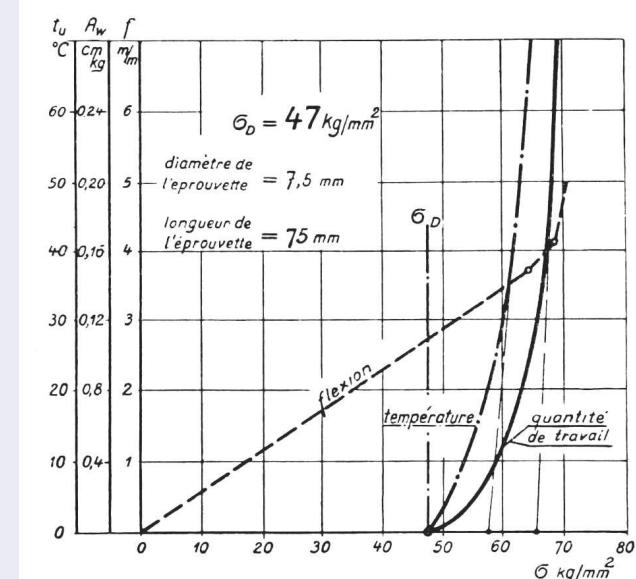


FIG. 59. — Variation de la flèche, de la température et de l'énergie absorbée en fonction de l'effort, au cours de la flexion rotative (LEHR).

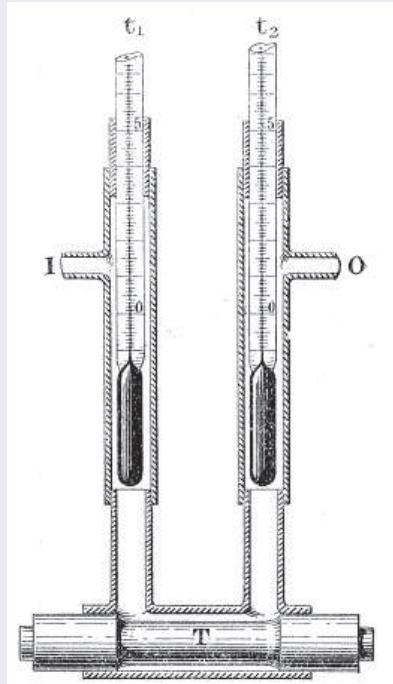
[Lehr and Skiba, Mot. Tech. Zeit., 1943]

## Self-heating tests

### *The Determination of Fatigue Limits under Alternating Stress Conditions.*

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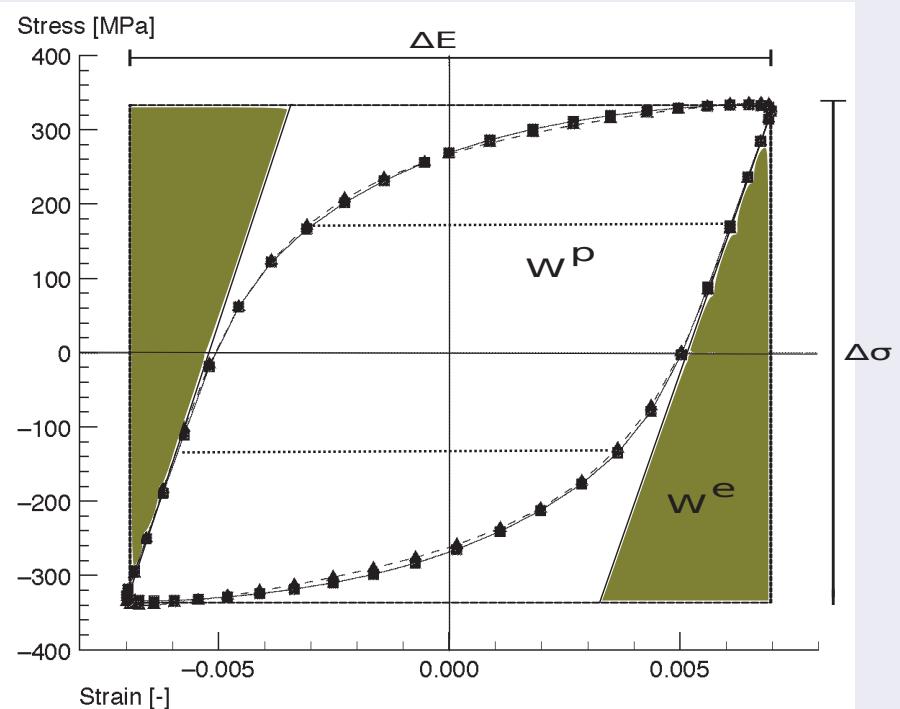


[Stromeyer, Proc. Roy. Soc., 1914]

### Fatigue limit and temperature

- What are the origin of such thermal variations?
- Is there a link with shakedown concept?
- Is there a link with fatigue damage?

## Cyclic loadings



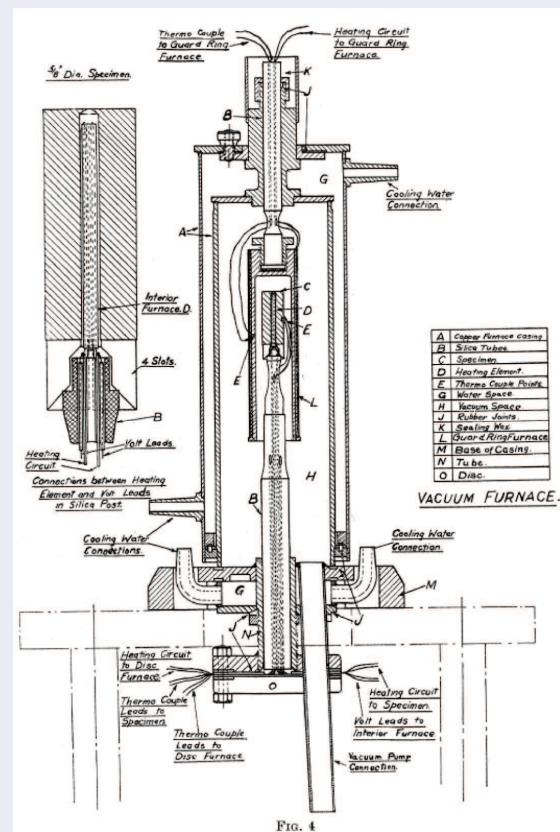
## A dissipative framework

- Inelastic strain energy → dissipation + storage
- Storage → Microstructural changes → Strain localization → Damage [Bever et al., Prog. Mat. Sci., 1973]

## Heat coupled equation in classical plasticity

$$\rho C \frac{dT}{dt} - \operatorname{div}(\underline{\underline{K}} \cdot \underline{\underline{\operatorname{grad}}}(\underline{T})) = \underbrace{(\underline{\underline{\sigma}} - \underline{\underline{X}}) : \dot{\underline{\underline{\varepsilon}}}_p - R \dot{p}}_{\text{intrinsic dissipation}} + \underbrace{T \frac{\partial \underline{\underline{\sigma}}}{\partial \underline{T}} : \dot{\underline{\underline{\varepsilon}}}_e}_{\text{thermoelastic coupling}}$$

## Calorimetry



[Quinney and Taylor, Proc. Roy. Soc., 1937]

$$\beta = 1 - \frac{d}{\sigma : \epsilon^p} \subset [5, 20] \%$$

## Infrared Thermography

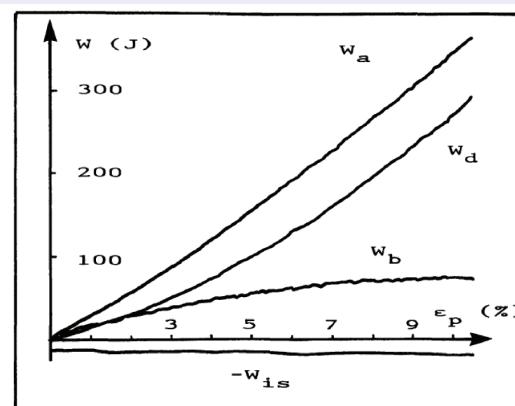


Fig. 6. — Bilan énergétique dans le cas d'un duralumin ; limitation de l'énergie bloquée.

[Energy balance in case of duralumin ; stored energy limitation.]

[\[Chrysochoos et al., Nucl. Engng. Design, 1989\]](#)

Classical constitutive laws are not "thermomechanically admissible", i.e. respect energy balance

## Towards the microstructure

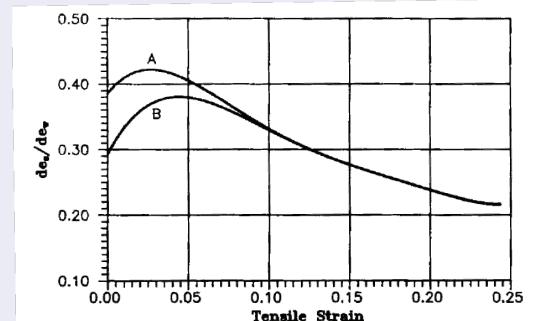
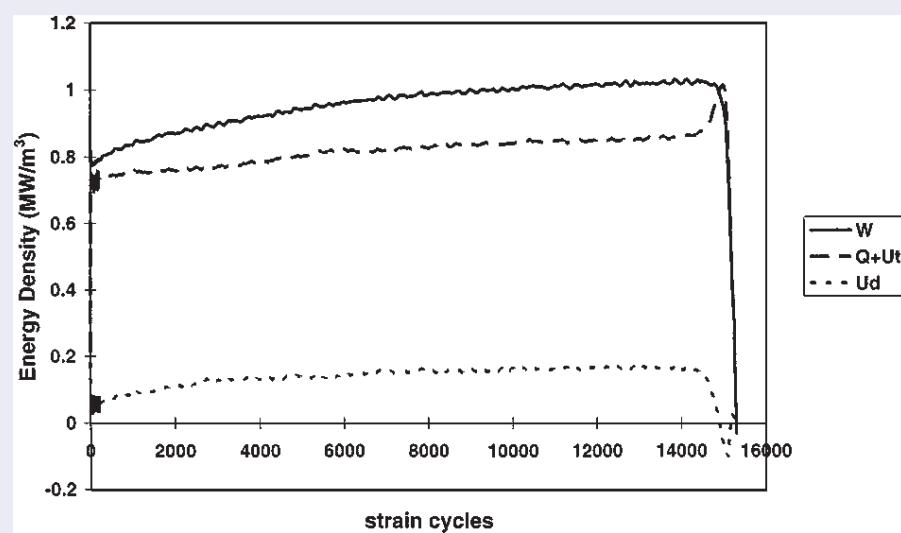


Fig. 7. Dependence of  $de_s/de_w$  vs. strain for the fine-grained (curve A) and coarse-grained (curve B) samples.

[\[Oliferuk et al., Mat. Sci. Eng. A, 1995\]](#)

$\beta$  depends on the microstructure  
(grain size ...)

## Macroscopic energy balance in fatigue

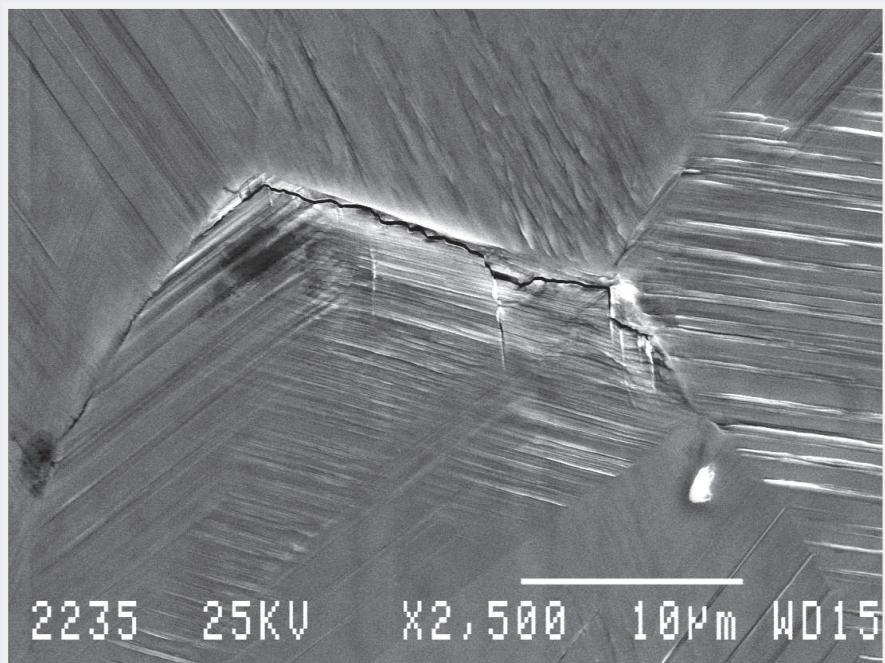


[Harvey et al., J. Mat. Sci. Lett., 2000]

## Fatigue process in polycrystals

- Polycrystal: grain aggregates with boundaries
- Crack initiation: PSB, GBs, TBs, defects...
- Local cyclic energy variations? **How?**  
**Where? Why?**

## Crack initiation in a AISI 316L stainless steel



[Sabatier, 2002]

## Fatigue process in polycrystals

- Polycrystal: grain aggregates with boundaries
- Crack initiation: PSB, GBs, TBs, defects...
- Local cyclic energy variations? **How?**  
**Where? Why?**

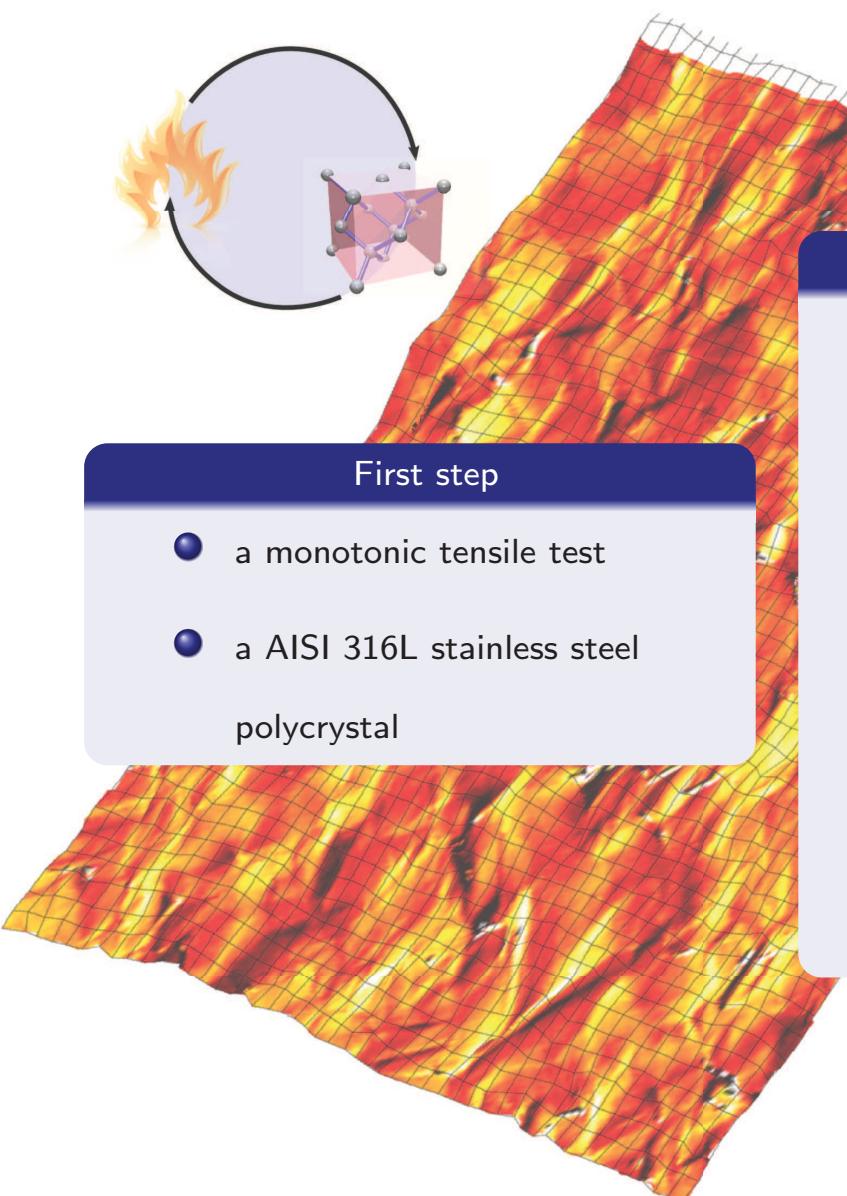
## Fatigue: an energy driven process?

- Can we see fatigue as an energy storage/release process?
- Does crack initiation correspond to a stored energy limit?

[Tanaka and Mura, J. Appl. Mech., 1981]

## Materials and methods

- A specific setup: ideally, **temperature**, stress and **strain** full-fields in polycrystals
- Single crystals, oligocrystals, **polycrystals**
- **Monotonic** tensile tests
- LCF tests
- HCF / VHCF tests

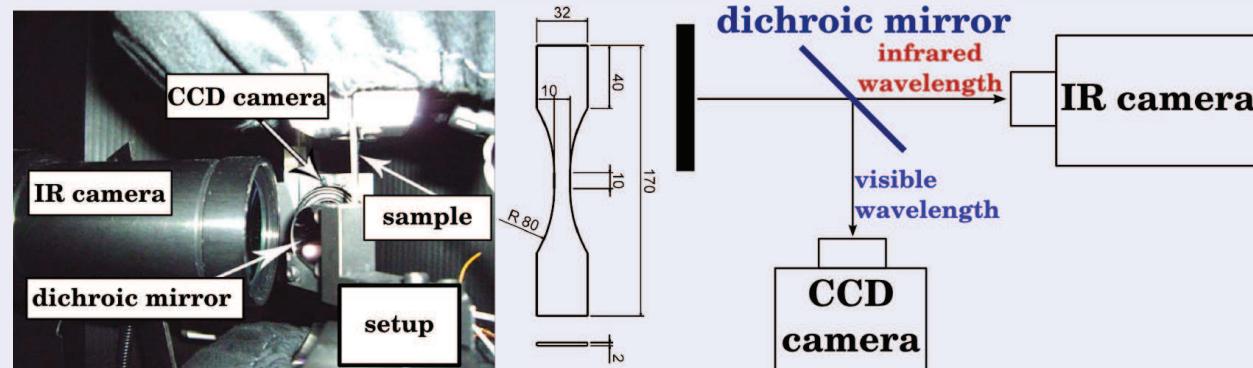


### Some requirements

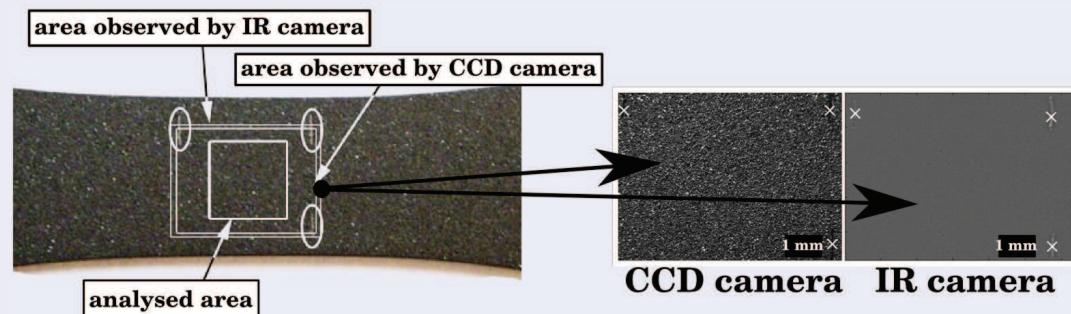
- 1 a specific test setup
  - *temperature and displacement fields at the grain scale*
- 2 multi-field analysis at the grain scale
  - *EBSD, profilometry, optical micrography*
- 3 calibration and treatment tools
- 4 internal variables
  - *Crystalline Plasticity F.E. strategy*

## An original test setup

Dichroic mirror able to separate infrared and visible wavelength



Specific coating adapted to Digital Image Correlation (speckle aspect) and thermal measurements (uniform aspect)



AISI 316L stainless steel heat treated for 2 hours at 1,200°C and water-quenched (mean grain size  $\approx 120\mu m$ )

[Bodelot et al., Mat. Sci. Eng. A, 2009] [Bodelot et al., Mech. Mat., 2011]

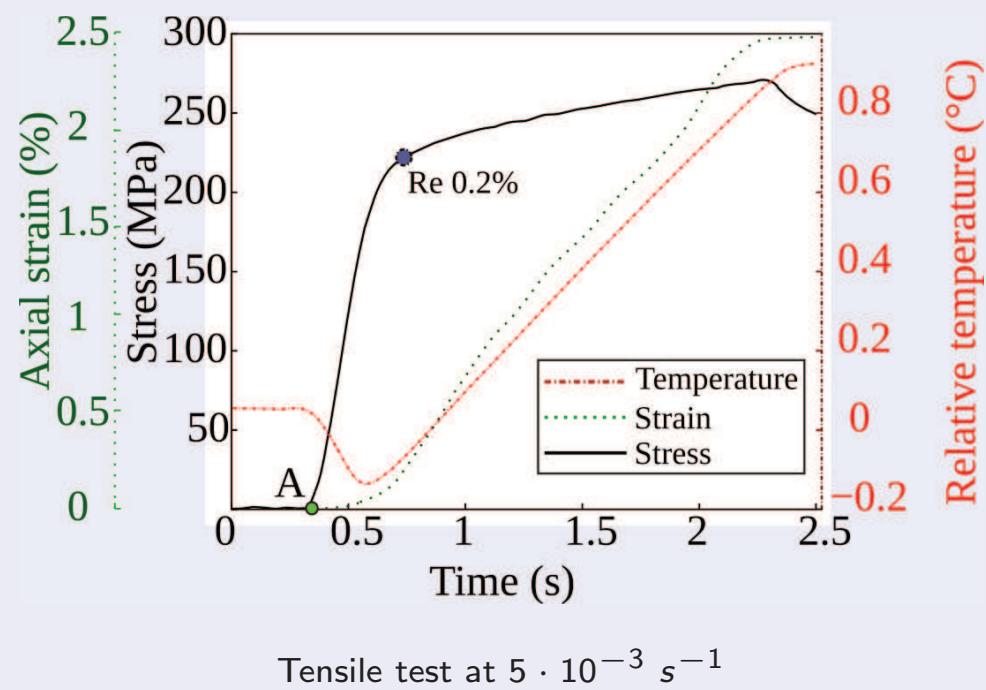
## A material and a test

Microstructure: 1,776 grains on surface



surface microstructure ( $5 \times 5 \text{ mm}^2$ )

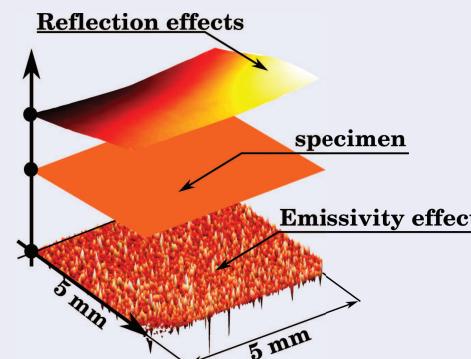
A monotonic tensile test



## Some specific developments



## A flux-based thermal calibration

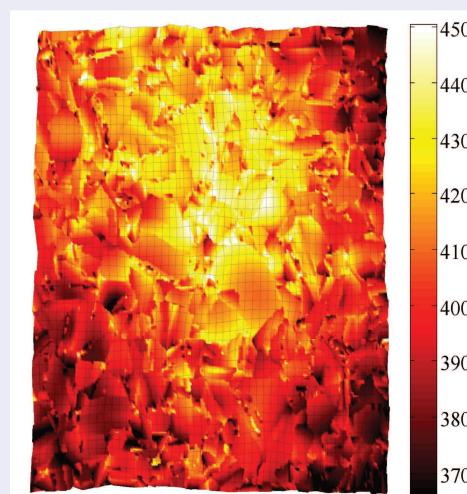


local emissivity map

from radiations to temperature

[Seghir et al., QIRT J., 2013]

## A data projection



first-order discontinuities

thermal and displacement fields

[Seghir et al., Mech. Ind., 2013]

## A thermoplastic simulation



internal variable estimation

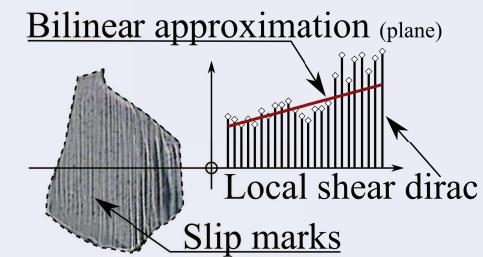
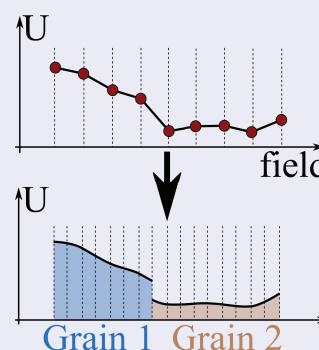
[Seghir et al., C. Mat. Sc., 2012]

### A crystallography-based projection

- 1<sup>st</sup> order discontinuity: grain boundary network
- piecewise continuous (intragranular domain)

### Assumptions

- assumes discontinuities at grain boundary: *Kapitza effect*, *strain incompatibilities* ...
- projection base
  - biparabolic displacement field per grain → bilinear strain field
  - biparabolic thermal field per grain → constant heat losses
  - analytic approach of intragranular domain
- additive decomposition (Field + Residue)

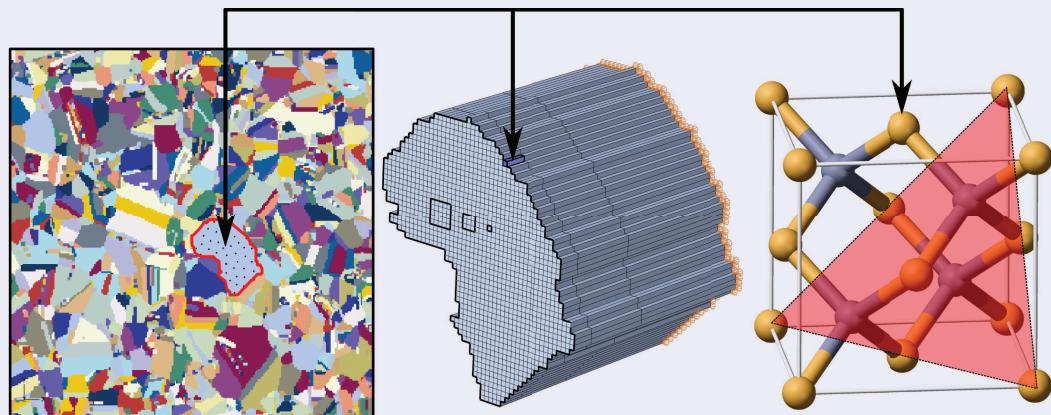


## Originality

crystalline plasticity and thermo-coupled  
finite element model

[Huang, Harvard University Report, 1991]

1,776 grains || DOF > 1,000,000 || 12 slip-systems CFC



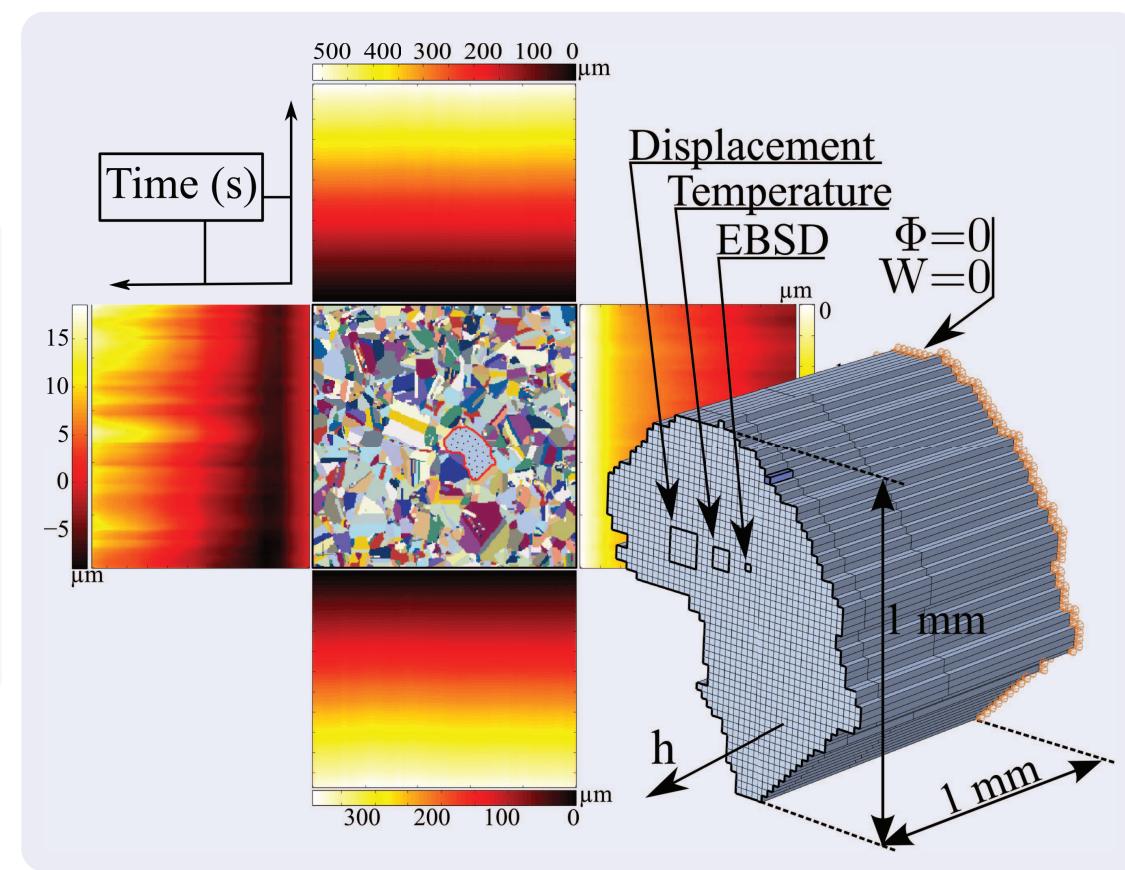
## F.E.M. and constitutive law

- Abaqus/standard and Fully Coupled Thermo-Mechanical calculation
- regular mesh (C3D8TR)
- dislocation density based (SSD)
- isotropic hardening (UMat)

## Crystal thermoplasticity framework

## Ingredients

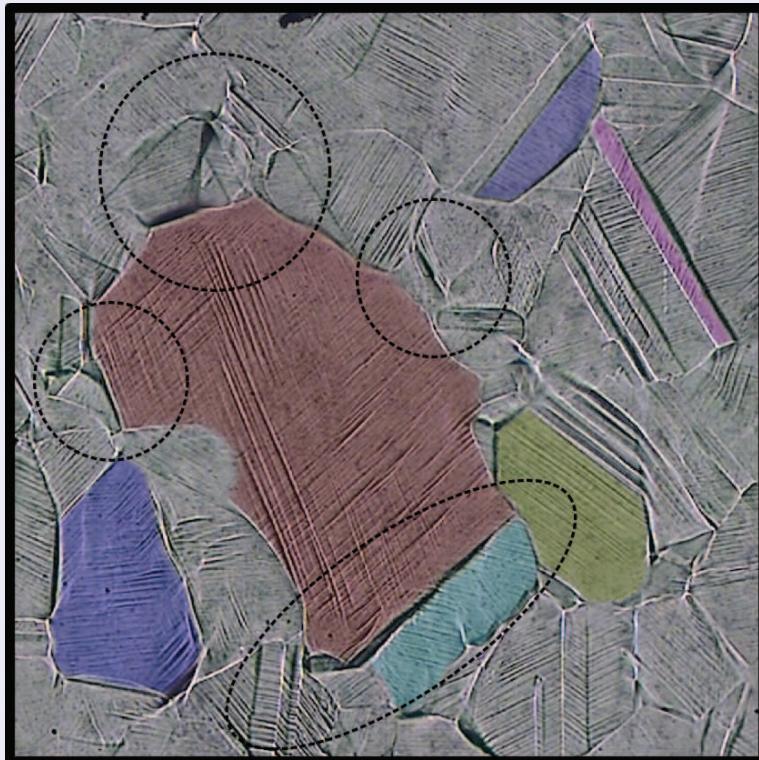
- $U_{exp}$  and  $T_{exp}$  at boundary nodes
- columnar boundary conditions
- symmetry on backface
- natural surface convection



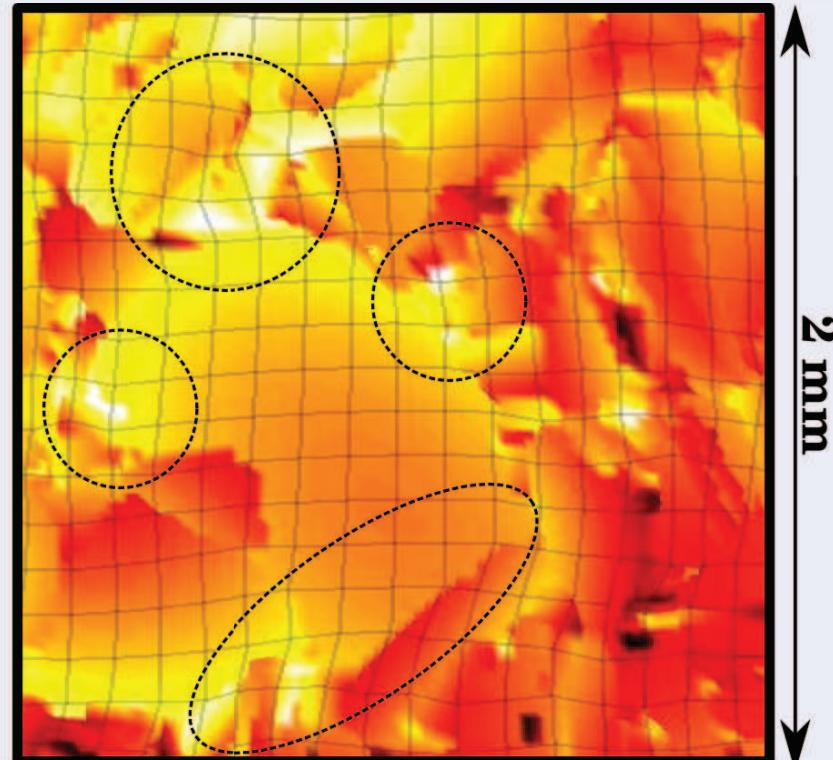
## Physical discontinuities

Importance of grain and twin boundaries [Kapitza, Phys. Rev., 1941]

surface micrography



temperature



## Fully coupled database

*Material*

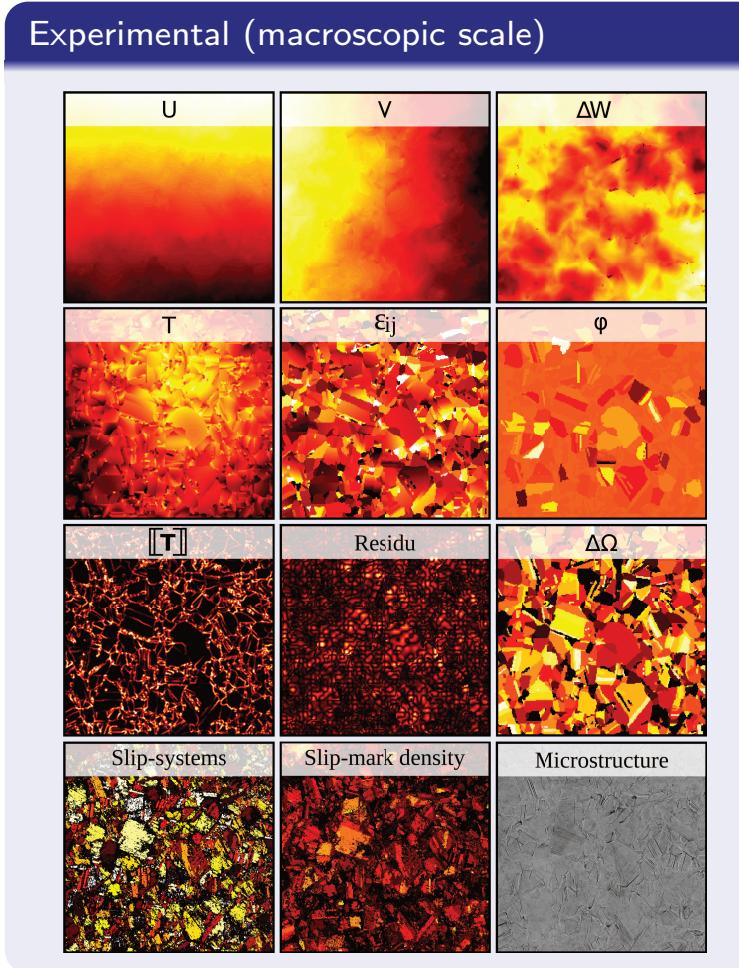
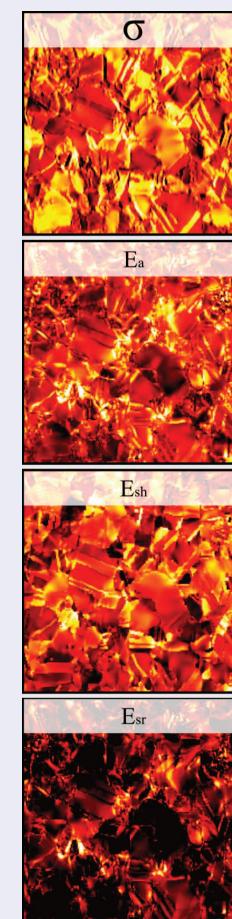
- AISI 316L
- grain<sub>Diam</sub> ≈ 120 μm

*Test*

- ε ∈ [0 → 2.5] %
- T ∈ [-0.17 → 0.8] K
- Zone: 5x5 mm<sup>2</sup>

*Resolutions*

- 104x104 μm<sup>2</sup>
- IR<sub>freq</sub>: 25 Hz
- IR<sub>res</sub>: 30 mK
- U<sub>freq</sub>: 7 Hz
- U<sub>res</sub>: 4x10<sup>-2</sup> μm

**Numerical (macroscopic scale)**

## Fully coupled database

Originality

intragranular heterogeneous

datas

Intragranular domain

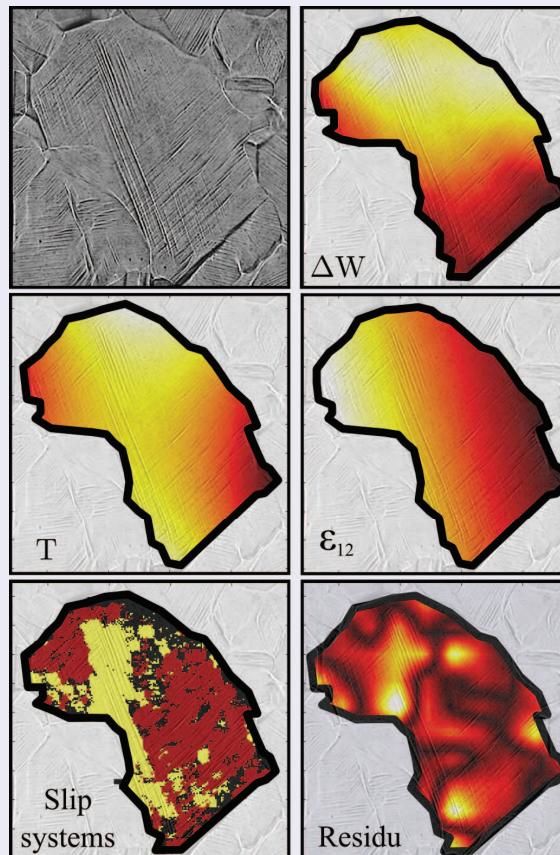
84% of grains >  $104 \times 104 \mu\text{m}^2$

$\mu\text{m}^2$

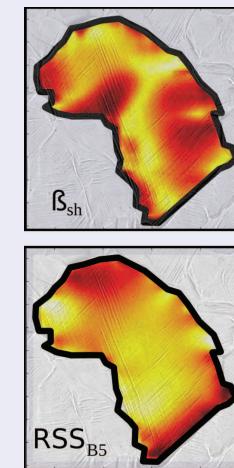
20 grains >  $400 \times 400 \mu\text{m}^2$

2 millimetric grains

## Experimental (intragranular scale)



## Numerical (intragranular scale)



Motivations

Experiment and data treatments

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Results and analysis

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Conclusions and prospects

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Multi-scale yield stress identification

## Multi-scale yield stress identification

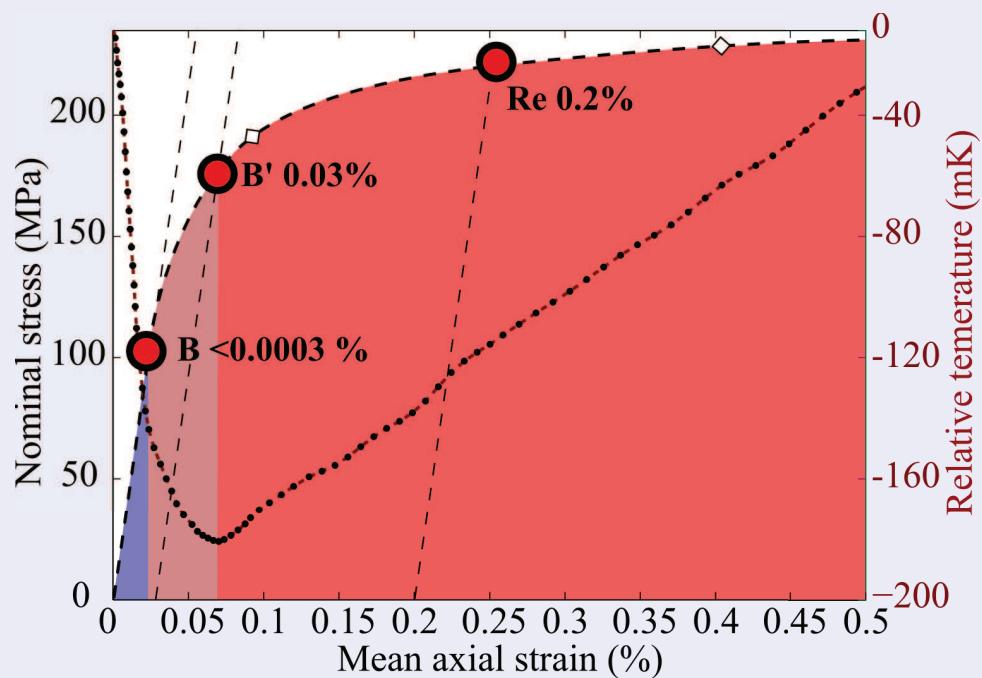
from macroscopic to intragranular plasticity

## Multi-scale yield stress identification: macroscopic scale

3 thermal phases

- 1 linear drop: *elasticity*
  - 2 inflection: *micro dissipation*
  - 3 increase: *global dissipation*
- [Lee, J. Mat. Sci., 1991]

## Macroscopic results



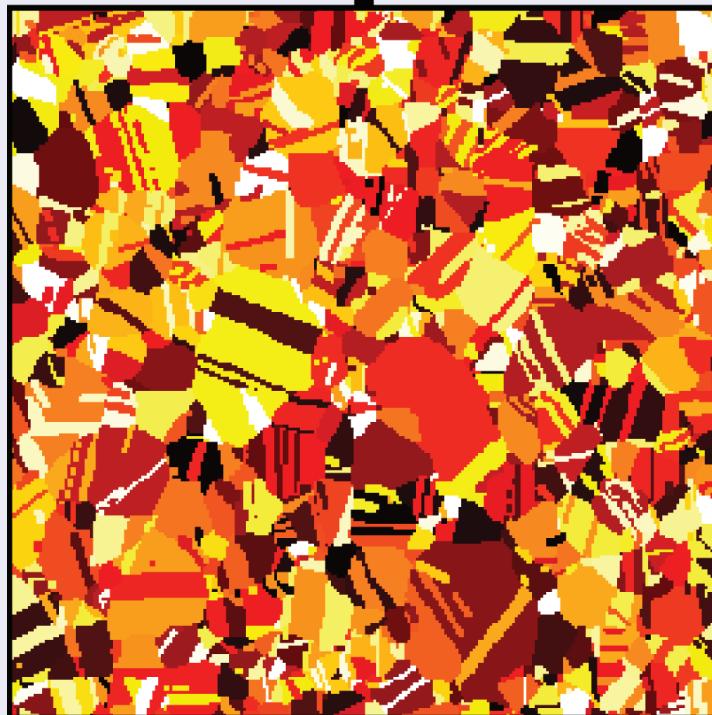
## Conclusion

**Identification of a macroscopic yield of dissipation  $\rightarrow \varepsilon^p < 10^{-4}\%$**

**by means of Maximum Likelihood method and deviation from thermal linearity**

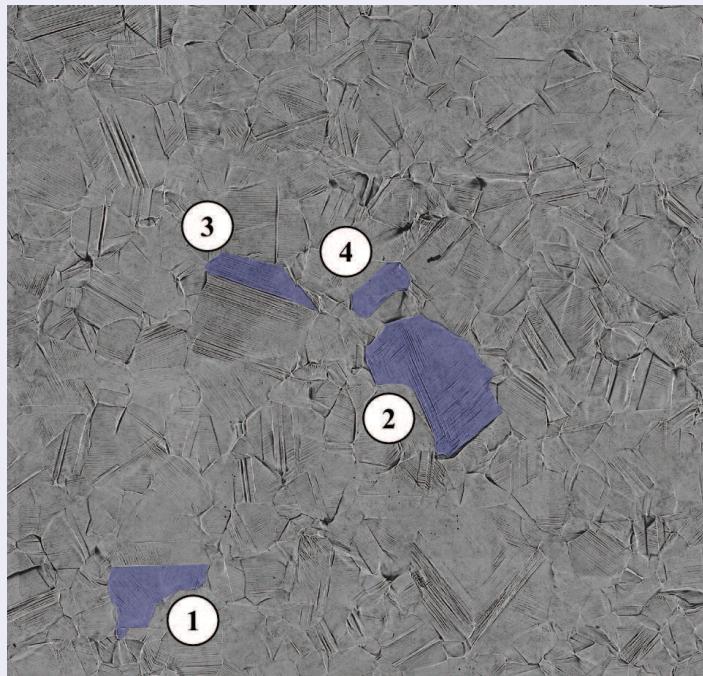
## Multi-scale yield stress identification: intragranular plasticity

$$\sum \uparrow E$$



## Multi-scale yield stress identification: intragranular plasticity

## Critical Resolved Shear Stress in individual grains

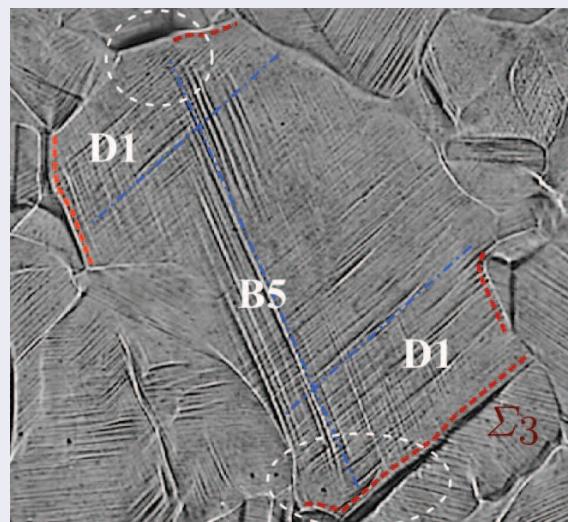


## Multi-scale yield stress identification: intragranular plasticity

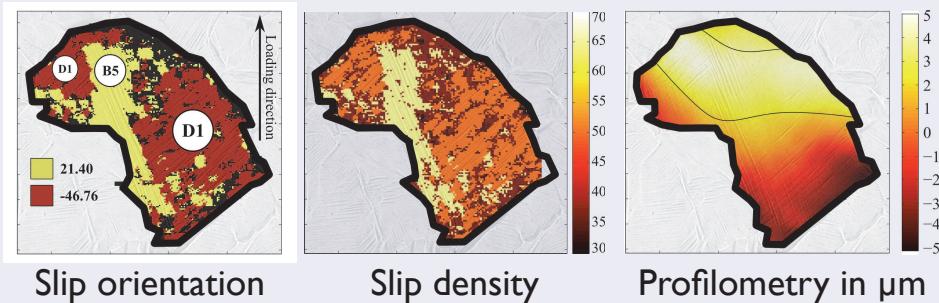
## Deformation scenario

2 distinct plastic domains  $D_1 \rightarrow B_5$ 

## Micrography



## Crystallographic point of view: slip-systems



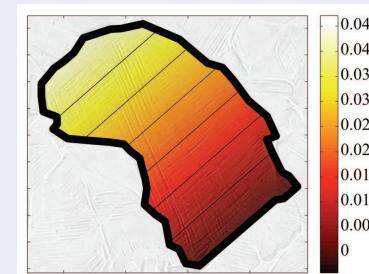
- significant impact of slip-systems on surface topography
- maximum Schmid factor principle: system  $D_1$  (0.339) then  $B_5$  (0.296)

## Multi-scale yield stress identification: intragranular plasticity

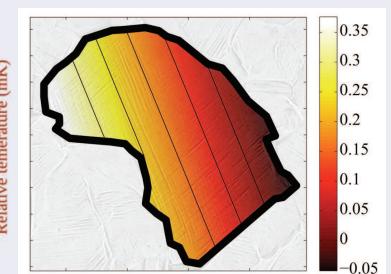
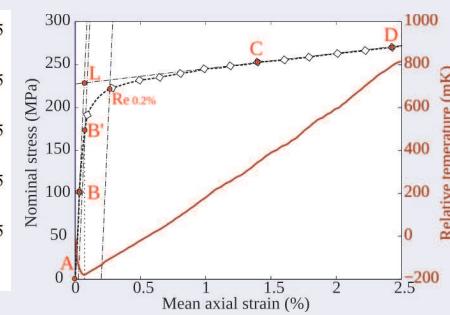
## Deformation scenario

- $D_1 < 106 \text{ MPa}$
- $191 < B_5 < 220 \text{ MPa}$
- $\tau_c = 35 \text{ MPa}$

$$\sigma = \mathbb{C}_{loc} : \epsilon^e \rightarrow \tau^s = \sigma : \mathbb{M}^s$$

Kinematic point of view:  $\varepsilon_{12}$ 

(B) system D1



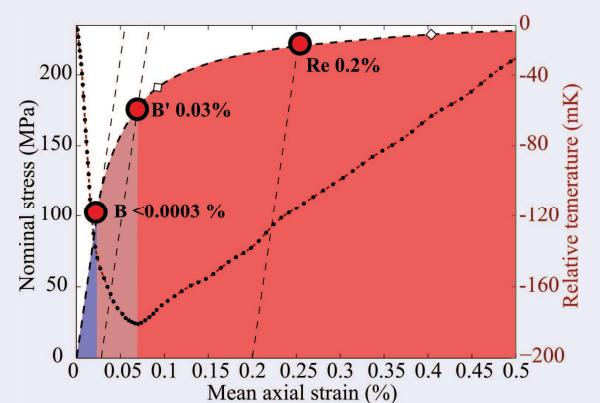
(Re 0.2 %) system B5

- in-plane slip isovalues in agreement with slip-marks orientations
- in line with Schmid theory: system  $D_1$  then  $B_5$
- no or neglectable multiple shear

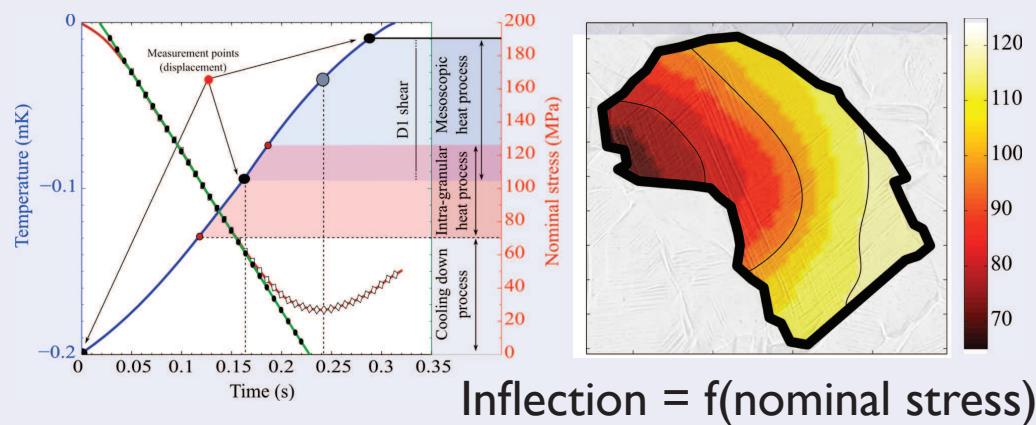
## Multi-scale yield stress identification: intragranular plasticity

## Deformation scenario

- kinematic  $\rightarrow \tau_c = 35 \text{ MPa}$
- $D_1$  dissipates early
- temperature  $\rightarrow \tau_c = 25 \text{ MPa}$



## Thermal point of view: local temperature inflection



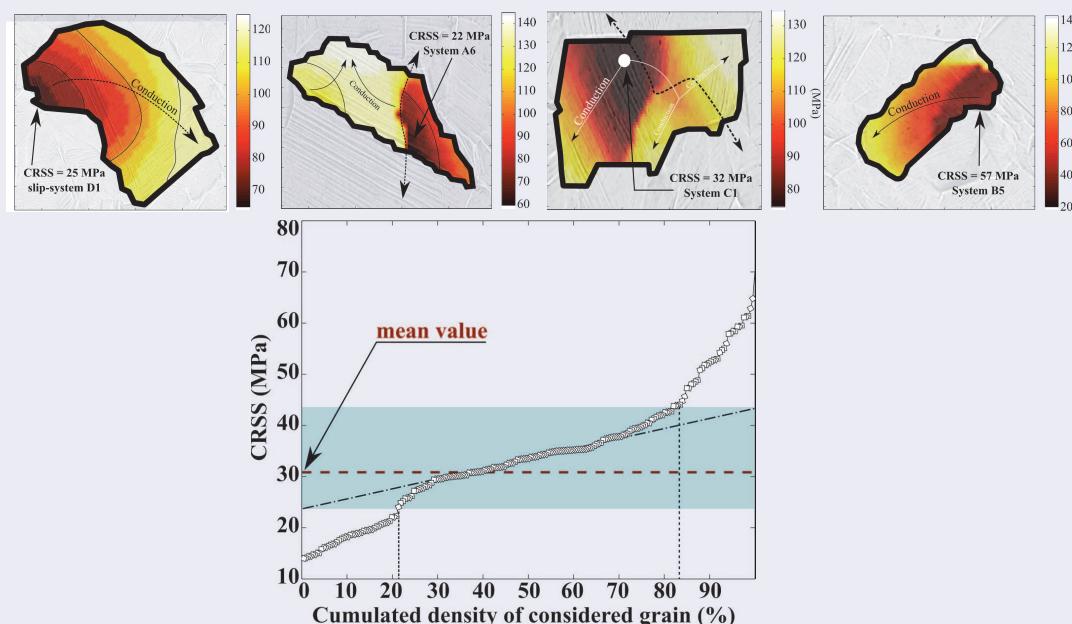
- intragranular thermal deviation from linearity at 78 MPa

## Multi-scale yield stress identification: intragranular plasticity

## Deformation scenario

- 2 distinct plastic domains  
 $D_1 \rightarrow B_5$
- kinematic  $\rightarrow \tau_c = 35 \text{ MPa}$
- temperature  $\rightarrow \tau_c = 25 \text{ MPa}$
- generalization:
  - grain diameter  
 $> 104 \mu\text{m}$
  - early inflection (165 grains)

## Statistical point of view: 165 grains



## Conclusion

**CRSS = 31 MPa  $\pm 7$  MPa within the polycrystal**

in line with [Feaugas, Adv. Eng. Mater., 2009] within AISI 316L single crystal

# Energy balance within polycristal

Intra- and intergranular stored energy

## Energy balance within polycrystals

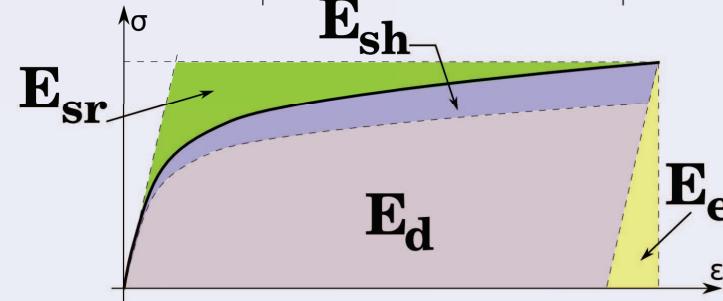
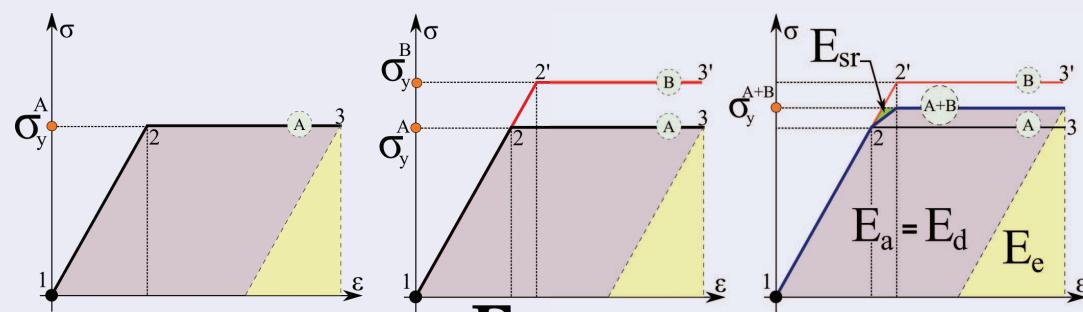
## Storage mechanisms in polycrystals

- 1  $E_{sr} \rightarrow$  stored elastic energy due to internal stresses field resulting from incompatibilities
- 2  $E_{sh} \rightarrow$  stored energy due to the hardening process (dislocations)

## Measurements

- 1  $E_s = E_{sh} + E_{sr} \rightarrow$  macroscopic energy balance
- 2  $E_{sr} \rightarrow$  stress-strain curve
- 3  $E_{sh} \rightarrow$  constitutive law

## Principle: elastic perfectly plastic bi-crystal



Polycrystals with local hardening

## Energy balance within polycrystal: macroscopic scale

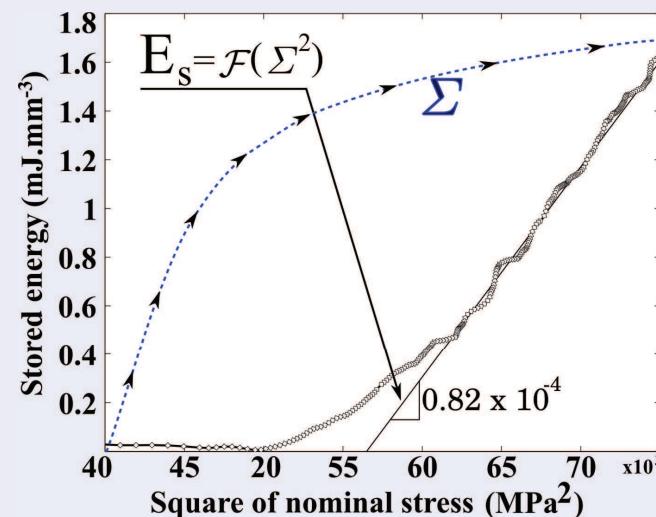
Theory: storage within dislocations only

$$E_s = \frac{m^2 \alpha_s}{\alpha^2 \mu} \Sigma^2 \approx 0.8 \times 10^{-4} \Sigma^2$$

[Schmid and Boas, 1950] [Bailey and Hirsch, 1960] [Williams, 1964] [Bever et al., 1973]

- $m$ : Schmid factor
- $\alpha$ : a constant  $\approx 0.3$
- $\alpha_s$ : a constant  $\in [1.8 - 2.1]$
- $\mu$ : the shear modulus

## Relation between stored energy and nominal stress

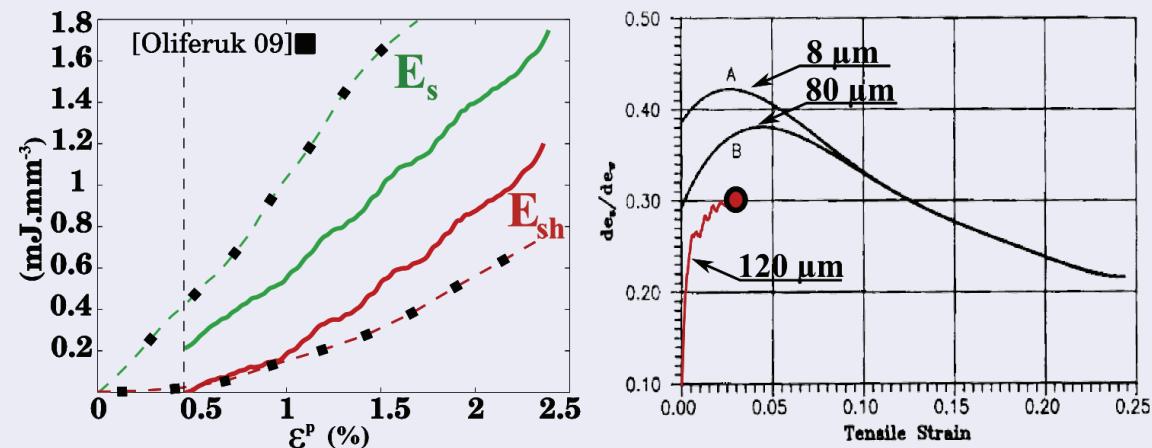


## Conclusion

linear hardening mainly due to dislocation

## Energy balance within polycrystal: macroscopic scale

## Macroscopic storage



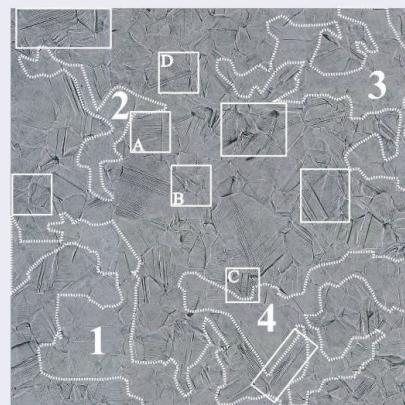
[Oliferuk et al., Eur. J. Mech. A/sol., 2009] & [Oliferuk et al., Mat. Sci. Eng. A, 1994]

## Observations

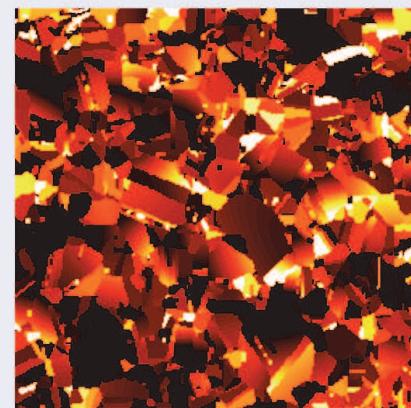
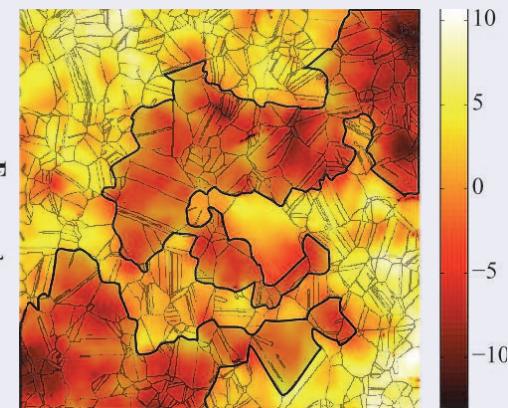
- confirmation: grain size  $\nearrow \beta^*$   $\searrow$  (early plasticity)
- observation at 2.5% of plastic strain:
  - grain size ( $\approx 20\mu\text{m}$ ): storage  $\rightarrow$  "internal stresses" 77%  $\rightarrow$  "hardening" 23%
  - grain size ( $\approx 120\mu\text{m}$ ): storage  $\rightarrow$  "internal stresses" 31%  $\rightarrow$  "hardening" 69%

## Energy balance within polycrystal: stored energy field

## Experimental estimation of stored energy



Micrography

 $E_s$  in ( $mJ \cdot mm^{-3}$ )

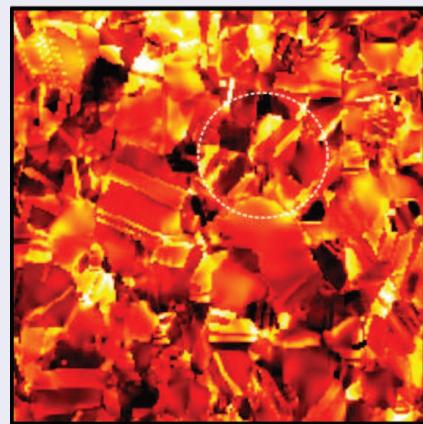
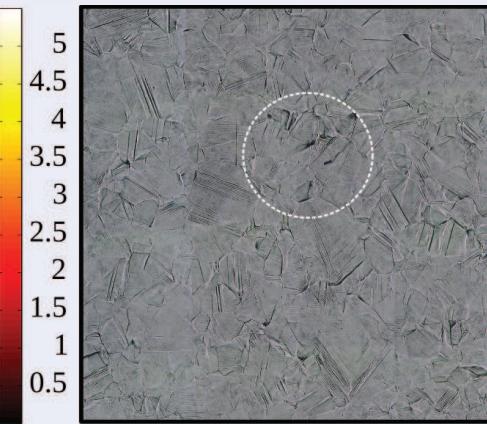
Profilometry

## Observations

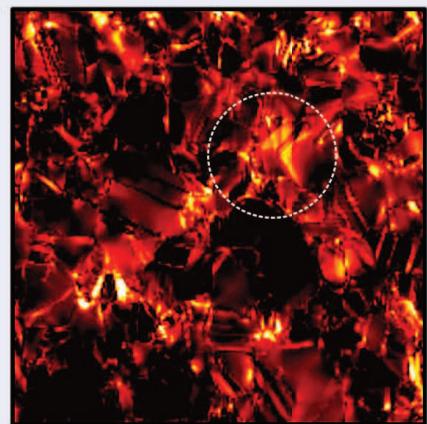
- $E_s$ : some intense vs. very low levels
- some qualitative relations with slip bands density: to be statistically improved

## Energy balance within polycrystal: stored energy field

## Numerical estimation of stored energies

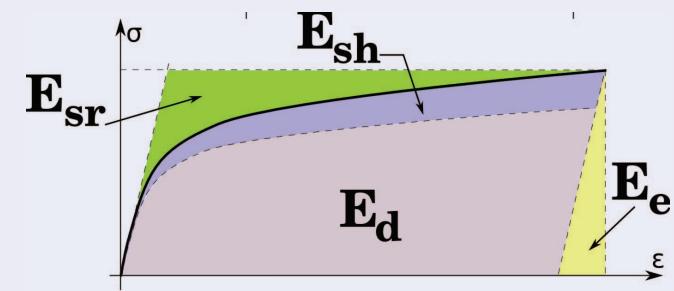
 $E_{sh}$  in ( $mJ.mm^{-3}$ )

Micrography

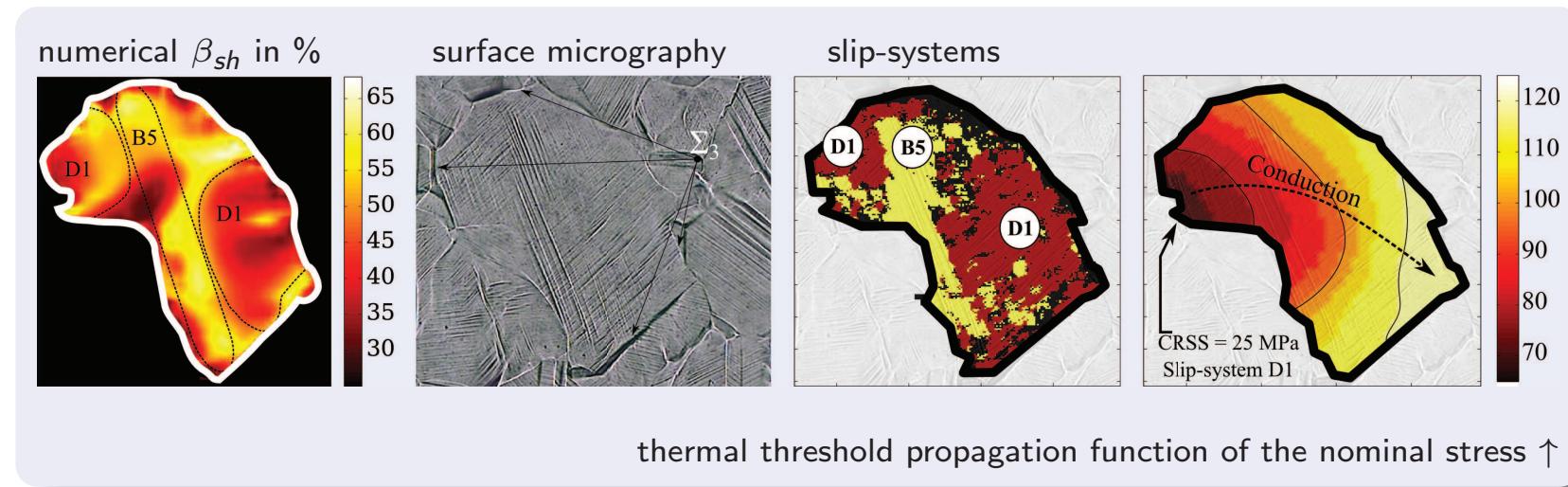
 $E_{sr}$  in ( $mJ.mm^{-3}$ )

## Observations

- $E_{sr}$  structural intense effect
- $E_{sh}$  intragranular plasticity effect



## Energy balance within polycrystal: intragranular stored energy



## Conclusions

- numerical results locally in line with experiment (millimetric grain)
- strong localization of  $\beta_{sh}^{num}$
- local level far from classical global ones (Taylor)
- interest of the local factor  $\beta_{sh}$  (localization indicator?)

## Thermomechanical couplings during the plastic deformation of polycrystals

## Conclusions

- 1 Multifields granular analysis on metallic polycrystal
  - surface temperature
  - strain tensor on surface
  - crystallographic orientations and grain geometry
  - slip bands intensity and orientation
  - profilometry ...
- 2 First steps on granular experimental and numerical thermomechanical analysis

## Prospects

- 1 Single crystals under monotonic and cyclic loadings
- 2 Role of the physical discontinuities (GBs, TBs, PSB ...)
- 3 Energy balance at the grain scale in fatigue?

## Thermomechanical couplings during the plastic deformation of polycrystals

Thank you for your attention

[eric.charkaluk@ec-lille.fr](mailto:eric.charkaluk@ec-lille.fr)