Effect of field fluctuations on the work-hardening of polycrystals

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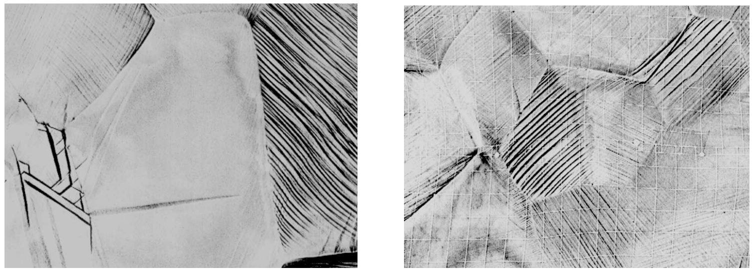
Outline

- Framework
- The model 2D polycrystal
  - Microstructure
  - Constitutive laws
- Full-field resolution by FFT
- Mean-field resolution using the S-C scheme
  - Classical work-hardening kinetic
  - New proposal taking into account fluctuations
- Conclusion & perspectives

Framework

Heterogeneous deformation of polycrystals



• SEM micrographs of a Zr alloy plastically deformed by uniaxial tension

- Inter- and intragranular plastic slip heterogeneities
- Associated fluctuations of the work-hardening

Framework

Considering a polycrystalline material, we aim at deriving by a *mean-field approach*

- its overall mechanical response
- its work-hardening at the *phase* scale

Phase: ensemble of grains with the same crystalline orientation.

Homogenization $\Longrightarrow$

∗ Description of the RVE ∗ Local law		∗ Overall behaviour ∗ Local fields

$\Longleftarrow$ Microstructure evolution

Objective: To take into account field fluctuations for the work-hardening description

Framework

Polycrystal made of N phases with K slip systems

$\dot{\gamma}_k$ and $\tau_{0\,k}$: *slip* rate and *critical shear* stress on slip system k

- *Local hardening law*

$$\dot{\tau}_{0\,k}(\mathbf{x}) = f(|\dot{\gamma}_1(\mathbf{x})|, |\dot{\gamma}_2(\mathbf{x})|, \ldots, |\dot{\gamma}_K(\mathbf{x})|), \quad \forall \mathbf{x} \in \text{phase } r$$

- *Averaging the hardening law*

$$\langle \dot{\tau}_{0\,k}(\mathbf{x}) \rangle_r = \langle f(|\dot{\gamma}_1(\mathbf{x})|, |\dot{\gamma}_2(\mathbf{x})|, \ldots, |\dot{\gamma}_K(\mathbf{x})|) \rangle_r = \quad ?$$

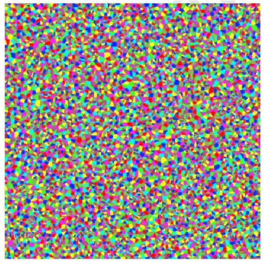
  - Requires informations on the slip rates distribution
  - Trivial cases: the Taylor and static models which assume uniform slip rates per phase

$$\langle \dot{\tau}_{0\,k}(\mathbf{x}) \rangle_r = \dot{\tau}_{0\,k}^{(r)} = f(|\dot{\gamma}_1^{(r)}|, |\dot{\gamma}_2^{(r)}|, \ldots, |\dot{\gamma}_K^{(r)}|)$$

Model 2D polycrystal

- Columnar orthorombic grains with crystal axis $\mathbf{e}_3$ // $\mathbf{x}_3$
- Two slip systems: (100)<001> and (010)<001>

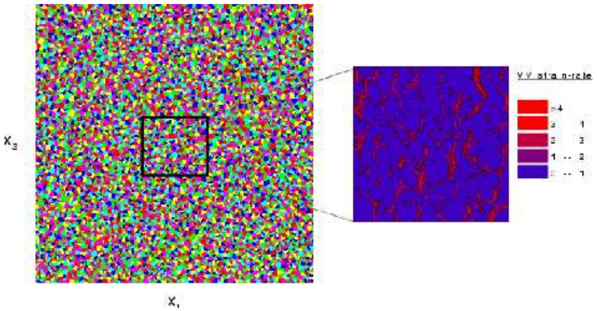
  $\dot{\gamma}_k(\mathbf{x}) = \dot{\gamma}_0 \frac{\tau_k(\mathbf{x})}{\tau_{0\,k}(\mathbf{x})}, \quad \dot{\tau}_{0\,k}(\mathbf{x}) = \sum_{k'} h_{kk'}(\mathbf{x}) |\dot{\gamma}_{k'}(\mathbf{x})|$
- Antiplane shear loading : $\dot{\bar{\varepsilon}}_{13}$
- 2D viscous constitutive relation : $\begin{pmatrix} \sigma_{13} \\ \sigma_{23} \end{pmatrix} = \begin{pmatrix} L_{1313} & L_{1323} \\ L_{1323} & L_{2323} \end{pmatrix} \begin{pmatrix} \dot{\varepsilon}_{13} \\ \dot{\varepsilon}_{23} \end{pmatrix}$
- Voronoi microstructure with 8500 grains and 8 crystalline orientations defined by $\theta = (\mathbf{e}_1, \mathbf{x}_1)$



FFT results

Fast Fourier Transform-based full-field formulation
(Moulinec and Suquet, 1994 – Lebensohn, 2001)

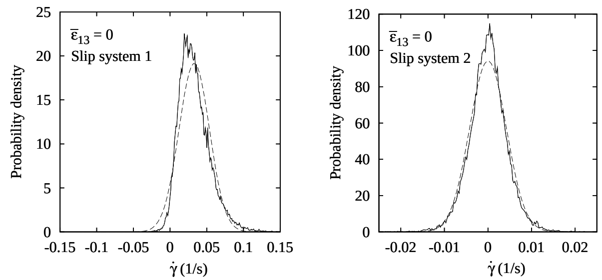
- Test conditions
  $\tau_{02}/\tau_{01} = 25$, $h_{kk} = 1\text{MPa}$, $h_{kk'} = 1.5 h_{kk}$ and $\dot{\bar{\varepsilon}}_{13} = 10^{-2}\text{s}^{-1}$
- Strain rate field



  - Tortuous localization bands running over several grains

FFT results

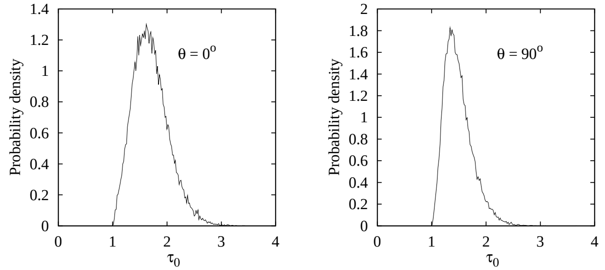
- Slip rates distribution ($\theta = 0°$)



  - System 1 : most active but presents locally a null or negative slip rate due to intergranular interactions
  - System 2 : null average but significant spread ⇒ contribution to work-hardening
  - Well approximated by Gaussian functions
  - Similar observations for the other phases

FFT results

- Reference stress distribution (Slip system 1)



  - Heterogeneity induced by the slip rates fluctuations
  - Asymmetrical distribution with a slowly decreasing tail
  - The “hard” phase (θ=90°) presents a smaller width

Mean-field approach

The self-consistent (SC) scheme is adopted in the following

- Local fields description
  - *Intraphase average* ⇒ By performing the average localization

$$\langle \boldsymbol{\sigma} \rangle_r = \langle \mathbf{B} \rangle_r : \bar{\boldsymbol{\sigma}}$$

  - *Intraphase fluctuation* ⇒ By taking the derivative of the overall energy with respect to phase compliances

$$\langle \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \rangle_r = \frac{1}{c_r} \left(\bar{\boldsymbol{\sigma}} \otimes \bar{\boldsymbol{\sigma}} \right) :: \frac{\partial \mathbf{M}}{\partial \mathbf{m}^r}$$

  - *Computational aspects*

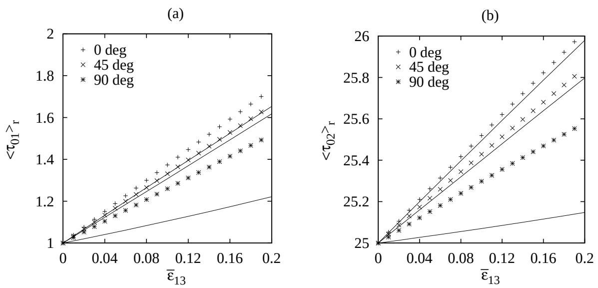
$\langle \boldsymbol{\sigma} \rangle_r$	Numerical integration of microstructural tensor $\mathbf{P}$
$\langle \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \rangle_r$	Construction of a linear system $\boldsymbol{\Delta} :: \partial \mathbf{M}/\partial \mathbf{m}^r = \boldsymbol{\Phi}^r$
	Additional numerical integration of $\partial \mathbf{P}/\partial \mathbf{M}$

Mean-field approach

- Classical procedure for hardening

  By neglecting the slip rates heterogeneity, it follows

$$\langle \dot{\tau}_{0k} \rangle_r = \sum_{k'} h_{kk'} |\, \langle \dot{\gamma}_{k'} \rangle \,|_r$$



  - A slip system with null average does not harden the material
  - Global underestimation of the hardening
  - Strong discrepancy for the “hard” phase ($\theta = 90°$)

Mean-field approach

- New proposal using slip rate fluctuations

  The average hardening law reads rigorously

$$\langle \dot{\tau}_{0k} \rangle_r = \sum_{k'} h_{kk'} \langle |\dot{\gamma}_{k'}| \rangle_r$$

  By assuming that the slip rates distributions are Gaussian, we obtain

$$\langle |\dot{\gamma}_k| \rangle_r = \mu \ \text{erf}(\beta) + \sqrt{\tfrac{2}{\pi}}\sigma \ \exp(-\beta^2)$$

  with $\mu = \langle \dot{\gamma}_k \rangle_r$, $\sigma = \left(\langle \dot{\gamma}_k^2 \rangle_r - \langle \dot{\gamma}_k \rangle_r^2 \right)^{0.5}$ and $\beta = \mu/(\sqrt{2}\sigma)$.

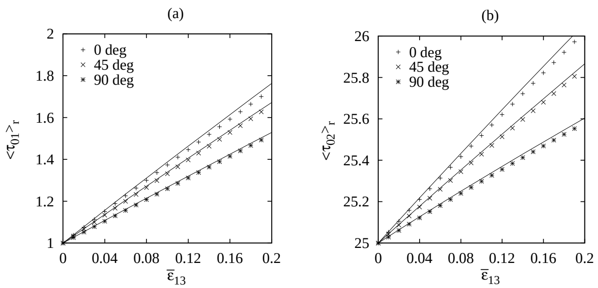
  The first and second moment of the slip rates are obtained by

$$\langle \dot{\gamma}_k \rangle_r = \dot{\gamma}_0 \left\langle \frac{\tau_k}{\tau_{0k}} \right\rangle_r \approx \dot{\gamma}_0 \frac{\langle \tau_k \rangle_r}{\langle \tau_{0k} \rangle_r}$$

$$\langle \dot{\gamma}_k^2 \rangle_r = \dot{\gamma}_0^2 \left\langle \frac{\tau_k^2}{\tau_{0k}^2} \right\rangle_r \approx \dot{\gamma}_0^2 \frac{\langle \tau_k^2 \rangle_r}{\langle \tau_{0k} \rangle_r^2}$$

Mean-field approach

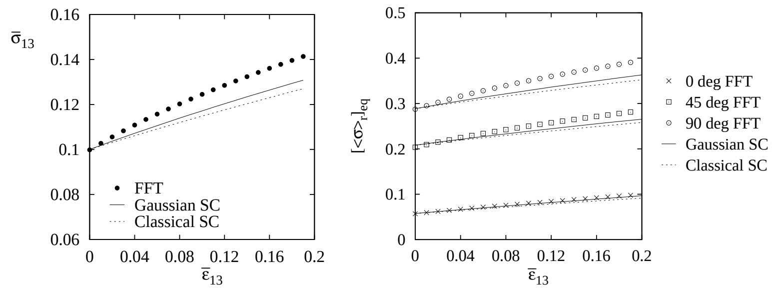
- Comparison with FFT results



  – Accurate description of the hardening kinetic
  – Clear improvement obtained for the hard phase

Mean-field approach

- Overall response and phase average equivalent stress



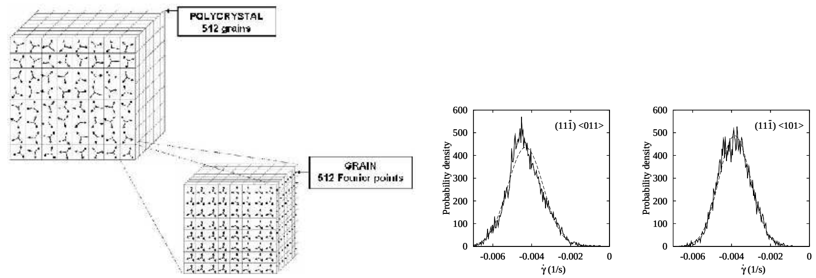
  – Improvement with respect to the classical procedure
  – Remaining discrepancy due to the fluctuation of τ_0 which is not correctly captured by the SC scheme

Conclusion

- The standard treatment fails to reproduce the average hardening kinetic
- The original method proposed, which accounts for the slip rates fluctuations, delivers the proper phase average of the local hardening law
- An additional assumption on the slip rates distribution is required
- The fluctuation of τ_0 within each phase gives rise to a specific hardening not captured by the self-consistent model

Work in progress

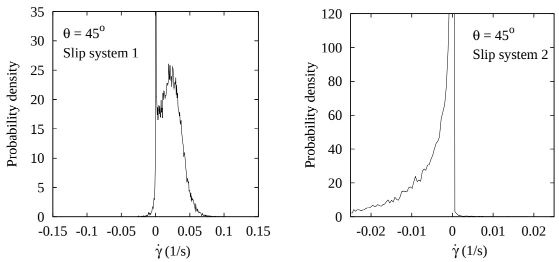
- Uniaxial tensile deformation of a linear 3D polycrystal



  – The Gaussian approximation still seems reasonable

Work in progress

- Nonlinear constitutive behaviour



  - Adequate choice of distribution functions ?
  - Use of an accurate nonlinear homogenisation procedure