Influence of the elastic anisotropy on the initial yielding of polycrystals

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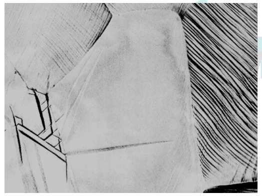
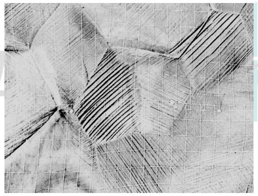
Outline

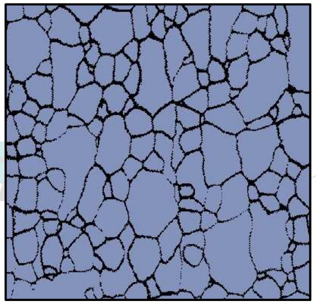
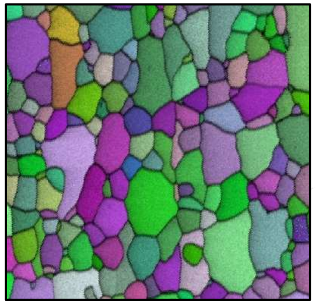
Motivation

Characterization of the local plastic response of polycrystals to understand elementary deformation mechanisms (micro-yield, slip/twinning activation, work-hardening etc.)

- Experiments : Microdiffraction setups ⇒ lattice distortion within grains
- Modelling : Full-field approaches (FEM, FFT, etc.) and homogenization estimates (self-consistent models)

How to define the micro-plastic onset of isotropic elastoplastic polycrystals ?

Isotropic elasticity	Anisotropic elasticity
	
Uniform stress field + Schmid law	Heterogeneous stress field + Schmid law
⇒ Tresca yield criterion	⇒ ?

(Grain color ⇔ local elastic behaviour)

Experimental observations:

- Operating slip systems with low Schmid factor
- Preferential slip activity near grain boundaries (Hashimoto and Margolin, 1983)

Modelling approaches:

- Self-consistent estimate of the micro-yield stress (Hutchinson, 1970)

  Shortcoming: elastic anisotropy leads to an increase of the yield stress !

- Numerous FEM studies of anisotropic elastic polycrystals

  Lack: link between stress fluctuations and micro-yield stress

Objectives:

- To derive new self-consistent estimates of the micro-yield stress
- To assess their relevance by comparison with a full-field modelling

FFT full-field method

Method conceived for periodic unit cells which makes use of Fast Fourier Transforms (Moulinec and Suquet, 1998)

Main features

- Heterogeneous medium $\Rightarrow$ Homogeneous medium ($\mathbf{C}^0$) with nonuniform polarization (τ)
- Iterative resolution of the Lippman-Schwinger equation

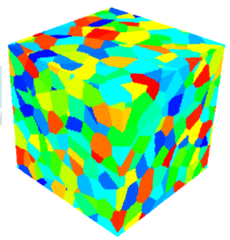
$$\varepsilon(\mathbf{x}) = \bar{\varepsilon} - \int_\Omega \mathbf{\Gamma}^0(\mathbf{x}-\mathbf{x}') : \tau(\mathbf{x}')\,d\mathbf{x}'$$

(Local relation in Fourier space)

- Images of the microstructure can be used as direct inputs (no meshing)
- Low numerical cost (CPU time and amount of memory required)

Construction of the unit cell

- Periodic Voronoi tesselation (500 cells)
- One crystalline orientation per cell
- Discretization into a regular grid



Discretization: $128 \times 128 \times 128$
Voxels per grain: ≈ 4200
Degrees of freedom: ≈ 6 millions

Ensemble averaging

- Statistical homogeneity and ergodicity
- Approximation of the RVE response

$\Downarrow$

Average over N_R realizations

Variability: volumic fraction, shape and spatial arrangement of grains

Example: Overall stress

Estimate:

$$\langle\sigma\rangle_{\text{RVE}} \approx \frac{1}{N_R}\sum_{i=1}^{N_R} \langle\sigma\rangle_{\text{UC}^i}$$

Relative error:

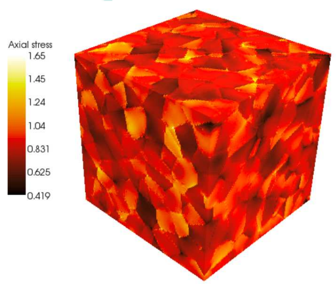
$$\delta = \frac{2\,\text{SD}(\langle\sigma\rangle_{\text{UC}})}{\sqrt{N_R}\,\langle\sigma\rangle_{\text{RVE}}}$$

3D elastic stress field

Constitutive behaviour: cubic elasticity (Zener parameter: $A = 2C_{44}/(C_{11}-C_{12})$)

Loading: uniaxial tension.

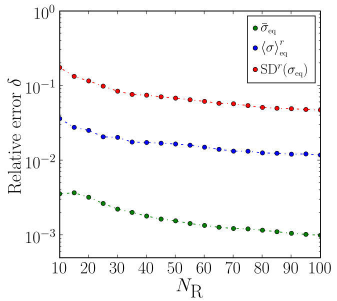
Example: case of Au polycrystal $\Rightarrow A = 2.8$



- Axial stress concentration factor (SCF) ranges from 0.4 to 1.6
- Preferential maxima close to grain boundaries

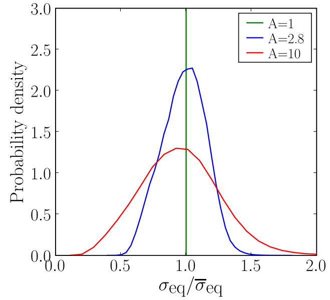
Representativity: which scale ?

Overall ? – Local average ? – Local fluctuations ?



- More than one order of magnitude between *overall* and *local* errors
- Convergence plateau depends on the discretization grid

Stress field distribution: effect of anisotropy



- Shape of the distributions close to Gaussian

The increase of the local anisotropy induces:

- the spread of the stress distribution
- the increase of the maximal SCF (right tail of the distribution)

Self-consistent model

Overall behaviour

- Exact estimate for *perfectly* isotropic, homogeneous and disordered polycrystals (Kröner, 1978)

Local fields

- Incomplete statistical description

Phase average: $\langle\varepsilon\rangle_r = (\mathbf{C}^r + \mathbf{C}^\star)^{-1} : (\widetilde{\mathbf{C}} + \mathbf{C}^\star) : \bar{\varepsilon}$

Phase variance: $\mathrm{VAR}^r(\varepsilon) = \underbrace{\langle\varepsilon\otimes\varepsilon\rangle_r}_{\frac{1}{c_r}\bar{\varepsilon} : \frac{\partial\widetilde{\mathbf{C}}}{\partial\mathbf{C}^r} : \bar{\varepsilon}} - \langle\varepsilon\rangle_r \otimes \langle\varepsilon\rangle_r$

N. B: Phase $r \equiv$ crystalline orientation

Which local criterion for plastic onset ?

Schmid law: the "local" resolved shear stress τ reaches a critical value τ_0

Full-field context

Local RSS ⇒ $\tau_k(\mathbf{x}^g) = \sigma(\mathbf{x}^g) : \mu_k^r$

Yield criterion ⇒ $\max_{\mathbf{x}^g} \max_k |\tau_k(\mathbf{x}^g)| = \tau_0$

$\mathbf{x}^g$: node of the regular grid – k: slip system – μ_k^r: Schmid tensor

Drawbacks:

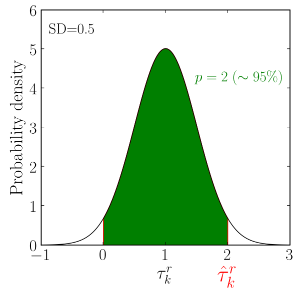
- High sensitivity to the discretization grid
- Requires many realizations for good accuracy
- Not transposable to other modelling approaches

Mean-field context

Proposition: statistical approach of the plastic onset

Reference RSS ⇒ $\hat{\tau}_k^r = |\langle\tau_k\rangle_r| + p\,\mathrm{SD}^r(\tau_k)$

Yield criterion ⇒ $\max\limits_r \max\limits_k \hat{\tau}_k^r = \tau_0$



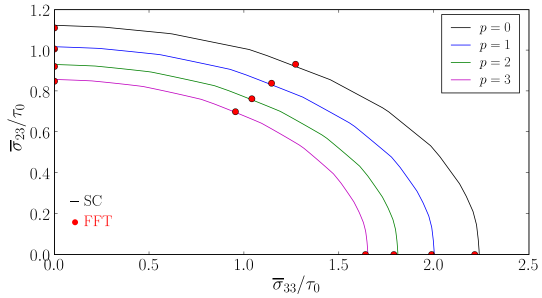
Features:

- Defines a *set* of probability yield surfaces ($p = 0, 1, 2, \dots$)
- Confidence interval ≡ % of the stress distribution entering the criterion
- Handy way to take into account stress fluctuations

Accuracy of the self-consistent estimates

Yield surface estimates in the tension-torsion stress plane

Zener parameter: $A = 2.8$

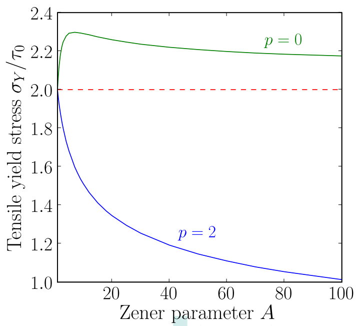


- Contraction of the yield surface estimate when $p \nearrow$
- Good agreement between SC and FFT for any p value
- No intrinsic drawbacks of the self-consistent model

Physical relevance of the yield criterion

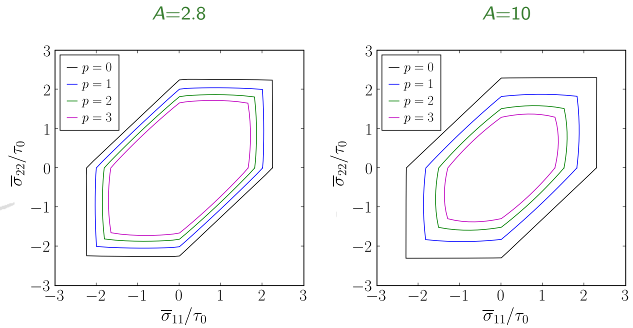
Evolution of the micro-yield stress with local anisotropy

- Drastically different trends with or without stress fluctuations in the yield criterion
- Incorporation of fluctuations leads to physically meaningful predictions:
  - σ_Y is below the Tresca yield stress
  - Monotonic ↘ of σ_Y when $A \nearrow$



(N.B: p=0 ⇒ Hutchinson's SC estimate)

Shape of the yield criterion



- The yield surface contraction increases with local anisotropy
- When stress fluctuations enter the yield criterion (i.e $p \neq 0$), the yield criterion deviates from a Tresca-type condition

Summary of the main outcomes

- Definition of initial yielding is not unique with the self-consistent scheme
- Novel statistical approach to describe the yield surface

- No intrinsic drawback of the self-consistent model
- Realistic estimates can be obtained if stress fluctuations are accounted for
- In general, the yield surface does not follow a Tresca-type criterion

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ratio $\sigma/2\tau_y^0$ and the abscissa is $E\epsilon/2\tau_y^0$ where ϵ is the total tensile strain. Thus, in this plot the elastic part of each curve has the same slope and the increase in the initial yield stress for the copper-like anisotropy above that of the isotropic case is evident.

The initial yield prediction of the self-consistent model must be qualified. A non-homogeneity in an elastic body usually acts as a stress raiser and tends to decrease, rather than increase, the stress at which plastic deformation first occurs. Single crystal anisotropy would be expected to have a similar effect; but according to the self-consistent model based on the spherical grain, it does not if

$$2C_{44} > (C_{11} - C_{12}).$$

The reason for this stems from the fact that stresses in each grain are calculated by treating it as a spherical inclusion. Stresses in the matrix surrounding the inclusion do not enter into the self-consistent estimate of initial yield. No doubt highly

Excerpt from "J. W. Hutchinson, *Proc. Roy. Soc. Lond* **A319** (1970), 247–272"