Some Variational Micro-Macro Models and their Application to Polycrystals

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- Recall : *Minimum and Maximum Work "Principles"*.

- Analysis of the development of several inhomogeneous micro-macro models derived from the Taylor model :

  "*Relaxed Taylor theory*", "*inhomogeneous Taylor model*",...

- Current state of *implementation of the proposed inhomogeneous variational model for polycrystals*.

Notation : $\boldsymbol{\sigma} = (\sigma_{ij})$, *microscopic* stress tensor (= in a grain)

$\mathbf{d} = (d_{ij})$, *microscopic* strain-rate tensor

$w(\mathbf{d}) = \boldsymbol{\sigma} : \mathbf{d} = \sigma_{ij}\, d_{ij}$, *rate of plastic work* (/volume)

$\boldsymbol{\Sigma}$, $\mathbf{D}$: *macroscopic* stress and strain-rate tensors

Recall : **Schmid law** (!)

1) $\exists$ *critical*, impassable values τ_k^c of the resolved shear stresses τ_k ;

2) prescribed *sign* of the shear rates : $\tau_k \,.\, \dot{\gamma}_k \geq 0 \quad \forall k = 1,\ldots,K$.

Taylor's (1938) Model =

* assumption of uniform strain-rate in the aggregate, $\mathbf{d}(\mathbf{x}) \equiv \mathbf{D}$

[just like Voigt (1887) for elasticity],

** Minimum internal work principle $\boldsymbol{\sigma} : \mathbf{d} = \sum_{k=1}^{K} \tau_k{}^c \, \dot{\gamma}_k = \text{Min}$

[data : **d** (for a "grain"; a priori , *no relation between* **d** *and* **D** !)

variables : shear rates $\dot{\gamma}_k$ $(k = 1,\ldots,K)$].

Bishop & Hill (1951) prove that :

1) Schmid law implies minimum work "principle".

2) Schmid law implies *maximum* work "principle", i.e.

$\boldsymbol{\sigma} : \mathbf{d}$ = Max [data: **d**, variable : $\boldsymbol{\sigma}$ admissible for the grain].

3) If $\overline{\boldsymbol{\sigma} : \mathbf{d}} = \overline{\boldsymbol{\sigma}} : \overline{\mathbf{d}} \left(= \boldsymbol{\Sigma} : \mathbf{D}\right)$, then maximum work passes to *poly*crystal.

4) If $\overline{\boldsymbol{\sigma} : \mathbf{d}} = \overline{\boldsymbol{\sigma}} : \overline{\mathbf{d}}$, Taylor ($\mathbf{d}^* \equiv \mathbf{D}$) provides an upper bound for

$$W(\mathbf{D}) = \boldsymbol{\Sigma} : \mathbf{D} = \overline{\boldsymbol{\sigma} : \mathbf{d}}.$$

In the **70** 's, *Taylor's model is implemented on computers.*

- Deformation textures : *approximately* it works !

  preferred orientations to 10° or more ;

  strongly overestimated maxima ;

  relative importance of preferred orientations poorly predicted.

  (e.g. cold-rolling of steel: Dillamore & Katoh 1974 (pencil-glide))

- Anisotropy coefficients (Lankford) overestimated.

  (e.g. steels : Bunge 1970, Parnière & Roesch 1975.)

=> Could no one find some better model than Taylor 's ?...

- Berveiller & Zaoui (1979) propose a simplified self-consistent model and begin to study its implementation.

- At the same time, some are looking for a model "closer to Taylor"...

Renouard & Wintenberger (1976) study theoretically the deformation of a *single crystal* subjected to *mixed* conditions ; thus,

(with L being some components *subset*, $L \subset [\{1,2,3\}\times\{1,2,3\}]_{sym}$,)

the data for the single crystal are :

$$d_{ij} = d_{ij}^0 \text{ for } (i, j)\in L, \quad \textit{and} \quad \sigma_{ij} = \sigma_{ij}^0 \text{ for } (i, j)\notin L.$$

They find that Schmid's law implies :

1) maximum work of *non-prescribed stresses*

$$\sum_{ij\in L} \sigma_{ij}\, d_{ij}^0 = \text{Max [variable: } \boldsymbol{\sigma} \text{ adm}^{\text{ble}} \text{ with } \sigma_{ij} = \sigma_{ij}^0 \text{ for } (i, j)\notin L]$$

2) (total work) *minus* (work done by *prescribed stresses*) = Min.

<u>Case $\sigma_{ij}^0 = 0$</u> for $(i, j)\notin L$: *minimum work*:

$$w(\mathbf{d}) = \text{Min [variable : } \mathbf{d} \text{ with } d_{ij} = d_{ij}^0 \text{ for } (i, j)\in L].$$

"Relaxed" Taylor model

(Honneff-Mecking 78, Kocks-Canova-Chandra 80-82, v Houtte 81-82)

One *assumes* that for a *polycrystal*, in *some cases* (e.g. rolling), one has

(RC) $\exists L : d_{ij} = D_{ij}$ for $(i, j)\in L$, *and* $\sigma_{ij} = \Sigma_{ij} = 0$ for $(i, j)\notin L$.

=> $\forall$grain, **d** makes $w(\mathbf{d})$ = Min among $\mathbf{d}^*$ with $d^*_{ij} = D_{ij}$ for $(i, j)\in L$.

Thus (RC) => actual **d** makes energy consumption the least.

"Inhomogeneous Taylor model" (Arminjon 1984)

Hypoth.: $\mathbf{d}$-$\mathbf{D} \in$ V bounded neighborhood of **0** tensor ;

for each grain *separately*, $w(\mathbf{d})$ = Min among $\mathbf{d}^*$ with $\mathbf{d}^*$-$\mathbf{D} \in$ V

NB1: For "relaxed Taylor" V={$\mathbf{d}^*$ with $d^*_{ij} = D_{ij}$ for $(i, j) \in$ L}

which is neither a neighborhood (too thin) nor bounded.

NB2: The simplest V: a ball, 1 parameter (radius r) fixes the model ;

Relaxed Taylor depends on a "discrete parameter" = subset L.

-Implementation (1987) => deformation textures well-predicted (steels).

2 param. δq et $\delta \phi$ (for technical reasons), found after 2-3 trials to simulate rolling texture of low C steels. Same values also work for other tested strain modes (uniaxial or biaxial tension,...) and for several low C steels with different microstructures.

- 1987: *Global* minimization proposed: $\overline{w(\mathbf{d})}$ = Min, $\bar{\mathbf{d}} = \mathbf{D}$, $\mathbf{d}$-$\mathbf{D} \in$ V.

Inhomogeneous variational model (Arminjon 1991):

General framework: statistically homogeneous medium with convex local potential $w = w(\mathbf{d}(\mathbf{X}), \mathbf{X})$ with $\mathbf{X}$ the local state, i.e., what makes the micro-law inhomogeneous (e.g. $\mathbf{X}$ = *crystal orientation*).

- "Constant-state averaged" fields are considered, e.g. $\mathbf{d} = \mathbf{d}(\mathbf{X})$.
- Volume average replaced by weighted average over the different states, e.g. $\langle \mathbf{d} \rangle := \int \mathbf{d}(\mathbf{X})\; f(\mathbf{X})\; d\mathbf{X}$ with f the ODF (for a polycrystal).

$h(\mathbf{d})$: the average inhomogeneity, $h(\mathbf{d}) := \langle \,|\, \mathbf{d} - \langle \mathbf{d} \rangle \,|\, \rangle$.

$W_r(\mathbf{D})$: the Min of $\langle w(\mathbf{d}) \rangle$ under constraints $\langle \mathbf{d} \rangle = \mathbf{D}$ and $h(\mathbf{d}) \le r$.

Theorem: *For any* $\mathbf{D}$, *there is one* $r_0 = r_0(\mathbf{D})$ *such that* $W(\mathbf{D}) = W_{r_0}(\mathbf{D})$

- If $r_0 = 0$, the Taylor model is correct, i.e. $\mathbf{d}(\mathbf{X}) \equiv \mathbf{D}$.
- If $r_0 \ge R(\mathbf{D})$ the "static" (Sachs) model is correct, i.e. $\boldsymbol{\sigma}(\mathbf{X}) \equiv \boldsymbol{\Sigma}$.

One problem is to find the *dependence* $r_0 = r_0(\mathbf{D})$ of the correct value. A phenomenological expression may be assumed: if it contains N parameters, then N tests will be needed to fix the model.

Application to fiber-reinforced mortars, a *strongly* inhomogeneous material ($\sigma_{\text{steel}}/\sigma_{\text{mortar}} = 600$) indicates that the simplest assumption:

$$r_0 = a\,|\mathbf{D}|\,,$$

allows to correctly predict the *macro-law*. Thus *one* parameter: a.

To find the *distribution* of **d** among different "grains" (orientations **X**), one assumes that the *solution* $\mathbf{d} = \mathbf{d}(\mathbf{X})$, such that $\langle w(\mathbf{d})\rangle$ is a Min under constraints $\langle \mathbf{d}\rangle = \mathbf{D}$ and $h(\mathbf{d}) \le r_0$, is indeed the *actual distribution*.

This amounts to a *"Principle of Minimal Inhomogeneity":*

$$h(\mathbf{d}) = \text{Min} \quad \text{under constraints } \langle \mathbf{d}\rangle = \mathbf{D} \text{ and } \langle w(\mathbf{d})\rangle = W(\mathbf{D}).$$

Thus (according to the model), *the inhomogeneity occurs only in so far as it allows to reduce the energy consumption*.

Implementation for polycrystal

(or other material with not-everywhere-smooth potential)

(new algorithm / algorithm used for fiber-reinforced mortar)

- Consider n constituents ("grains") $k = 1,\ldots, n$ with volume fractions f_k

- Condition $\langle \mathbf{d} \rangle \equiv \sum_{k=1}^{n} f_k \, \mathbf{D}^k = \mathbf{D}$ accounted for by eliminating n^{th} grain

  => variable $\mathbf{Y} = (\mathbf{D}^{*k})_{k=1,\ldots,\underline{n-1}}$

- Functional to be minimized (convex, but not strictly convex) :

$$F(\mathbf{Y}) \equiv \sum_{k=1}^{n} f_k \, W_k(\mathbf{D}^{*k}) \ .$$

(W_k : rate of work [or potential] in constituent N° k)

under (not strictly) convex inequality constraint

$$h(\mathbf{Y}) \equiv \sum_{k=1}^{n} f_k \left| \mathbf{D}^{*k} - \mathbf{D} \right| \leq r_0$$

Unless r_0 is too large, solution is *not* the static one: $\boldsymbol{\sigma}^k$ not all equal.

Then the inequality constraint may be changed to *equality constraint*.

- Solution always exists and non-uniqueness should be exceptional.

- Constraint $h(\mathbf{Y}) = r_0$ accounted for by the penalty method:

to find $\mathbf{Y}$ making $F(\mathbf{Y})$ = Min under constraint $h(\mathbf{Y}) = r_0$, solve

$$F_1(\mathbf{Y}) \equiv F(\mathbf{Y}) + \rho\,[h(\mathbf{Y}) - r_0]^2 = \text{Min}, \qquad \rho >> 1,$$

Rmk: one has

$$\frac{\partial F}{\partial \mathbf{D}*^k} = f_k \left(\frac{\partial W_k}{\partial \mathbf{D}*^k} - \frac{\partial W_n}{\partial \mathbf{D}*^n} \right) = f_k \left(\boldsymbol{\sigma}^k(\mathbf{D}*^k) - \boldsymbol{\sigma}^n(\mathbf{D}*^n) \right),$$

so it is clear that Min without constraint <=> static model ($\boldsymbol{\sigma}^k = \boldsymbol{\sigma}^n\ \forall k$)

- Conjugate gradient method (2nd derivatives not analytical + irregular)

- Directional minimization: Newton method + modified dichotomy.

- Pb. near "static" model (no constraint): only the weakest constituent is deformed. But the potential F is irregular at $\mathbf{Y}=(\mathbf{D}^k)$ if $\exists\ \mathbf{D}^k = 0$.