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Self-consistent large strain modeling of polycrystals: Application to ductility loss prediction

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Abstract

The elastic-plastic behavior of polycrystals is studied. A single-crystal constitutive law is defined thanks to crystalline plasticity in the large strain framework. The self-consistent scheme is adopted to obtain macroscopic behavior from microscopic one. Rice's criterion is introduced to predict ductility loss. Obtained results show the proposed model ability to simulate single-crystal and single-phase polycrystals behavior. It can also give good qualitative results on forming limit diagrams prediction.

Key words: ductility, crystalline plasticity, self-consistent modeling, forming limit diagram

1 Introduction

Micro-macro methods are more and more used to compute heterogeneous materials behavior. Their main interest resides in the computation of stress/strain behavior but also texture evolution, lankford coefficient, etc... Those methods have been widely studied. They generally consist of two parts:

- Firstly, the definition of the local law which can have several forms depending on the type of behavior considered. Here, the rate independant

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crystalline plasticity from previous works already published in [2], [1] and [8] is taken as the local constitutive law.
- Secondly, the link between the local behavior and the global one which is called the scale-transition method. Many schemes have been developed, from the most simple like Taylor [18] or Sachs [17] ones to more complicated ones. The self-consistent scheme introduced by Berveiller and co-workers [4] from earlier work of Eshelby [5] and Kröner [9] has been chosen.

The obtained macroscopic elastic-plastic model is coupled to a ductility loss criterion in order to be able to predict numerically forming limit diagrams. To do that, the first part of this paper will be focused on the local law, the second part on the self-consistent scheme and the third part on the introduction of Rice's criterion [16]. Once the proposed model is entirely defined, the results for single crystal and single-phase polycrystals in terms of stress/strain behavior are given. Finally, Rice's criterion is used to give qualitative results on ductility loss.

2 Modeling

2.1 Single crystal modeling

2.1.1 Hypotheses

In order to model the single crystal behavior some assumptions have been made:

- The description is made within the large strains framework,
- Elastic strains remain small,
- Rate-independent behavior,
- The plastic strain is only due to slip over crystallographic planes. Other mode of deformation like twinning or phase transformation are not considered.
- The behavior law between nominal stress rate $\dot{n}$ and the velocity gradient g is assumed to be an incremental one : $\dot{n} = l : g$ where l is the fourth order tangent modulus and : defines the double contracted product of tensors.

2.1.2 Strain decomposition

Only main lines of the single crystal constitutive law are here recalled. More details have already been published [11]. It is assumed that the velocity gra-

dient g can be decomposed into a symmetric part d and a skew one w as:

$$g = d + w \tag{1}$$

The tensor d can be decomposed into an elastic part with the superscript e and a plastic part with the superscript p. It is the same for the rate of total lattice rotation w. By the introduction of Schmid's tensors R^g and S^g and the slip rate $\dot{\gamma^g}$ acting on the slip system g one has:

$$d = d^e + d^p = d^e + \sum_g R^g \dot{\gamma^g} \tag{2}$$

$$w = w^e + w^p = w^e + \sum_g S^g \dot{\gamma^g} \tag{3}$$

2.1.3 Active slip system determination

The classical formulation for the active slip system determination is:

$$\begin{aligned} \tau^g_{res} < \tau^g_c &\Rightarrow \dot{\gamma^g} = 0 \\ \tau^g_{res} = \tau^g_c, \dot{\tau}^g_{res} < \dot{\tau}^g_c &\Rightarrow \dot{\gamma^g} = 0 \\ \tau^g_{res} = \tau^g_c, \dot{\tau}^g_{res} = \dot{\tau}^g_c &\Rightarrow \dot{\gamma^g} \geq 0 \end{aligned} \tag{4}$$

Where τ^g_c and τ^g_{res} define respectively the critical and the resolved shear stress acting on the system g. Many possible sets of slip systems are solution of (4). To choose the real active set of slip systems, a criterion based on an energetic minimization [6] was adopted. It induces a high computing cost (a combinatory analysis is needed). To avoid this, a new formulation based on mathematical regularization functions is introduced. It can be written in the form:

$$\dot{\gamma^g} = k^g \dot{\tau}^g_c \tag{5}$$

With:

$$k^g = \frac{1}{8H^{gg}} \left(1 + th\left(k_0 \tau^g_{res}\right)\right) \left(1 + th\left(k_1 \left(\frac{\tau^g_{res}}{\tau^g_c} - 1\right)\right)\right) \left(1 + th\left(k_2 \dot{\tau}^g_{res}\right)\right) \tag{6}$$

Where H^{gg} is the self hardening parameter, k_0, k_1 and k_2 are numerical parameters whose typical value are respectively 1, 20 and 1. The gain of computing time over a classical analysis is about 98%.

2.1.4 Fourth order tangent modulus

By introducing elasticity within the large strains framework thanks to the fourth order elastic tensor C , the fourth order tangent modulus is given by

(with summation over g and h):

$$l = \left(C - \frac{1}{2}\left(\delta \star \delta\right).\sigma - \frac{1}{2}\left(\delta \diamond \delta\right).\sigma\right) - \left(C : R^h + S^h.\sigma - \sigma.S^h\right)\left(\delta_{gh} + k^g R^g : C : R^h\right)^{-1} : k^g R^g : (C - \sigma \otimes \delta) \quad (7)$$

Where δ is the Kronecker symbol, . defines the simple contracted product, $\otimes$ denotes the tensorial product,

$$\left(\delta \star \delta\right).\sigma = \left(\delta_{ik}\delta_{lm} + \delta_{il}\delta_{km}\right)\sigma_{mj} \text{ and } \left(\delta \diamond \delta\right).\sigma = \left(\delta_{jk}\delta_{lm} - \delta_{jl}\delta_{km}\right)\sigma_{mj} \quad (8)$$

To complete the description of the model, definition of the hardening matrix where mean dislocation density acting on each slip system is taken as internal variable can be found in [3]. Internal variable evolution can be found elsewhere [11]. Since the description of the local law is given, the scale transition scheme can be applied to obtain the macroscopic elastic-plastic behavior.

2.2 Scale transition

The macroscopic velocity gradient and nominal stress rate are the volume average of the local ones:

$$\dot{N} = \frac{1}{V}\int \dot{n} dV \qquad and \qquad G = \frac{1}{V}\int g dV \quad (9)$$

Then, it is assumed that the global behavior can be described thanks to a law in the same form as the local one (where N, G, L are the macroscopic nominal stress, velocity gradient and tangent modulus).

$$\dot{N} = L : G \quad (10)$$

The self-consistent scheme has been introduced in order to determine the strain concentration tensor A^I of the grain I linking the macroscopic velocity gradient to the local one. The calculus of this tensor has been made by Lipinski [10], its expression is:

$$A^I = \left(I - T^{II}\left(l^I - L\right)\right)^{-1} : \left(\frac{1}{V}\int_V \left(I - T^{II}\left(l^I - L\right)dV\right)\right)^{-1} \quad (11)$$

Where T^{II} is the interaction tensor. The self-consistent tangent modulus is given in the case of ellipsoidal grains of volume fraction f^I as:

$$L = \sum_I f^I l^I : A^I \quad (12)$$

When the tangent modulus loses its ellipticity, instability can occur [14]. This is well determined by Rice's criterion [16] which is detailed in the next paragraph.

2.3 Ductility loss criterion

The authors have chosen to use Rice's criterion in order to detect strain localization because of its simplicity and this is a three-dimensional criterion. In the present model the authors have not taken into account any structural aspect of the material which does not allow to introduce Considère's or Hill's criterion. The assumption of this criterion is that, when localization occurs, a band, each part of whose mecanichal fields are no more continuous is created. The formulation of this criterion is:

$$det\left(\nu_i L_{ijkl} \nu_k\right) = 0 \tag{13}$$

Where ν is a vector defining the normal to the localization band. Because the behavior law relates nominal stress rate to velocity gradient this formulation is frame-independant and valid within the large strain framework.

3 Results

3.1 Behavior modeling

Numerical results to predict single crystal and polycrystal behavior are given Fig. 1 and Fig. 2. In each series of tests, only four parameters need to be identified. For the others, classical values for steels are taken [11]:

- The initial critical resolved shear stress acting on each slip systems family.
- The critical annihilation distance.
- A parameter linked to the mean free path of dislocations.

Fig. 1 presents the simulation of several shear tests on Fe-Si single crystal on the plane (1-10) extracted from Rauch [15]. All parameters are fitted on the test with the direction [110]. They remain constant for the other tests which are simulated by only changing Euler's angle by their respective values. This figure shows a good agreement between the numerical results labelled "th" and the real ones labelled "exp". It can be seen, that, in each case elastic limit and hardening slope are correctly predicted. This valids the efficiency of the proposed model in predicting the influence of crystallographic orientation on the behavior. Fig. 2 presents the simulation of a low-carbon ferritic intersitial

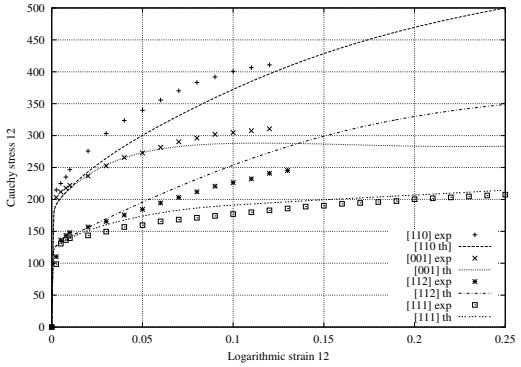

Fig. 1. Single crystals shear tests

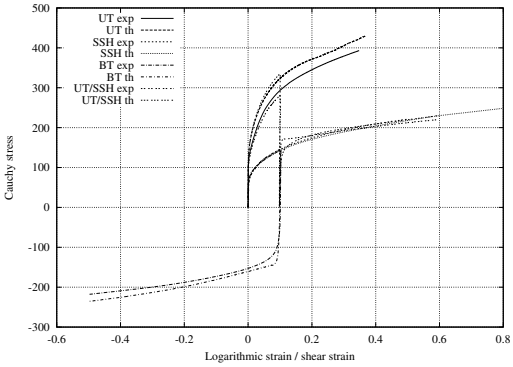

Fig. 2. Polycrystal behavior prediction

free steel. The same labels as in Fig. 1 are used. The abbreviations on the figure are UT for uniaxial tension, SSH for simple shear, BT for Bauschinger test and UT/SSH for uniaxial tension then shear test. The parameters are here identified for the shear test then, as before, remain constant for the others. It has to be noted that the initial measured texture is an input of the model. This figure shows also a good agreement between numerical and experimental results. But, at the onset of the second test during complex loading path, there is a large difference between numerical and experimental tests. It is due to the dislocation microstructure created during the first loading. This microstructure needs to be "broken" in order to create another corresponding to the second path [13]. Those discrepancies are explained by the fact that no dislocation microsctructure is taken into account.

3.2 Ductility limit prediction

Fig. 3 presents the effect of the initial critical resolved shear stress on the ductility limit. It gives the strain level corresponding to ellipticity loss of the macroscopic tangent modulus vs the initial critical resolved shear stress. This curve shows that the higher the elastic limit is, the lower the ductility, which seems to be a good qualitative result. It can be compared with the work of Luft [12], who has made tensile tests on molybdenum single crystal at various temperatures. The variation of temperature make a change on the elastic limit (the lower the temperature, the higher the elastic limit) which have the same effect on ductility than in Fig. 3. Fig. 4 presents forming limit diagrams for the same material as in Fig. 2. In the curve labelled "stress conditions" all the components of the macroscopic stress tensor are imposed. In the one labelled "coupled conditions" the macroscopic strain is imposed in the sheet plane and the other components are stress controled. This figure shows that the obtained curves have the right shape but the wrong level of strain (lower than the experimental one) [7]. The difference could be explained by the fact that, in this model, no structural effect is taken into account. The localization point is, in fact, the first point of the material where localization occurs. But

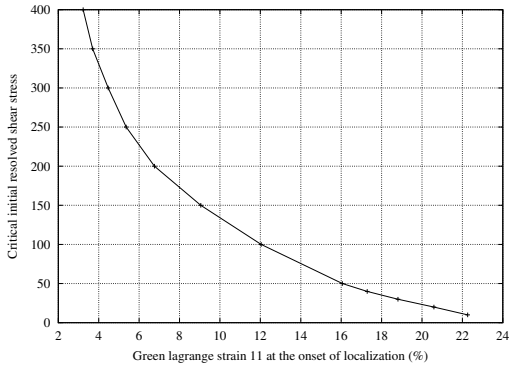

Fig. 3. Elastic limit influence on ductility

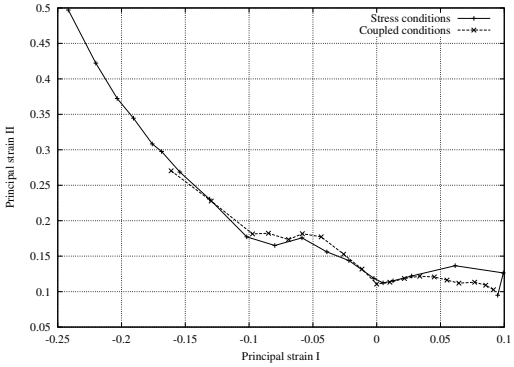

Fig. 4. Polycrystal forming limit diagram

experimental data are taken when a localization band is visible, which can also explain the difference with numerical results.

4 Conclusions

In this paper a self-consistent large strain model has been presented. It has been shown that:

- The crystalline plasticity model used is able to predict the behavior of single-crystals.
- The self-consistent scheme applied to the crystalline plasticity is able to predict the behavior of a polycrystal for single and complex loading paths.
- The introduced ductility criterion gives good qualitative results for the single crystal in term of elastic limit influence. The polycrystal forming limit diagram can be drawn with the right shape in comparison with experimental results.

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