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Strain localization analysis deduced from a large strain elastic-plastic self-consistent model for multiphase steels

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Abstract: In order to investigate the impact of microstructures and deformation mechanisms on the ductility of materials, the criterion based on bifurcation theory first proposed by Rice is applied to elastic-plastic tangent moduli derived from a large strain micromechanical model combined with a self-consistent scale transition scheme. This approach takes into account several microstructural aspects for polycrystalline aggregates: initial and induced textures, dislocation densities, softening mechanisms so that the behavior during complex loading paths can be accurately described. Based on this formulation, Forming Limit Diagrams (FLDs) are derived and compared with a reference model for multiphase steels involving linear and complex loading paths. Furthermore, the effect of various physical and microstructural parameters on the ductility limit of a single-phase steel is qualitatively studied with the aim of helping in the design of new materials.

1. Introduction

Nowadays, FLDs are commonly considered at localization since the onset of localized necking is the main limitation of industrial forming processes. During sheet metal forming processes, several failure modes may occur (buckling, wrinkling, diffuse and localized necking) and may sometimes even be coupled with damage phenomena. As a unified approach taking all these mechanisms into account seems to be very difficult, the present work only focuses on the onset of strain localization due to macroscopic shear band formation.

The main objective of this work is to predict the loss of ductility of multiphase steels with maximum accuracy by taking into account the impact of changing loading paths and mechanical properties with the aim of designing new materials. For this purpose, a criterion introduced by Rudnicki and Rice [1] (see also Rice [2]) and based on the formation of strain localization bands corresponding to jumps of mechanical fields across interfaces, will be coupled with a constitutive law derived from a large strain micromechanical approach and a self-consistent scale transition scheme. Comparisons with experiments, for several direct as well as sequential rheological tests, are presented for two multiphase steels. A detailed strain localization analysis is carried out, which allows us to conclude on the relationship between microstructure and ductility.

2. Multiscale model

2.1. Single crystal modeling

First, it is necessary to define the assumptions from which the elastic-plastic single crystal behavior will be modeled. The plastic deformation is assumed to be only due to crystallographic slip; the other plastic deformation modes like twinning or phase transformation are not considered. The single crystal constitutive modeling is valid for both B.C.C. and F.C.C. materials. In this paper, only B.C.C. steels are studied. Therefore, there are 24 independent slip systems for B.C.C. crystals which are given by the two families $\langle 1\ 1\ 1 \rangle (1\ 1\ 0)$ and $\langle 1\ 1\ 1 \rangle (1\ 1\ 2)$. This model is dedicated to the investigation of sheet forming steels, what supposes modeling the behavior within the large strain framework. The local incremental elastic-plastic constitutive law gives the relation between the nominal stress rate $\dot{\mathbf{n}}$ and the velocity gradient $\mathbf{g} = \frac{\partial \mathbf{v}}{\partial \mathbf{x}}$ through the tangent modulus \mathbf{l} as:

$$\dot{\mathbf{n}} = \mathbf{l} : \mathbf{g} \quad (1)$$

The developed model is based on the pioneering contributions of Asaro and Rice [3], Asaro [4], Pierce [5], Pierce *et al.* [6], see also Iwakuma and Nemat-Nasser [7], in which a new criterion for the determination of the set of active slip systems and a new formula for the slip rate calculation are proposed [8,9].

The total strain rate \mathbf{d} (symmetric part) and the total rotation rate \mathbf{w} (skew-symmetric part) of the velocity gradient $\mathbf{g} = \mathbf{d} + \mathbf{w}$ can be split into an elastic part with the superscript e and a plastic one with the superscript p . The plastic parts are related to the slip rates $\dot{\gamma}^g$ by:

$$\begin{aligned} \mathbf{d}^p &= \mathbf{d} - \mathbf{d}^e = \sum_g \mathbf{R}^g \dot{\gamma}^g \\ \mathbf{w}^p &= \mathbf{w} - \mathbf{w}^e = \sum_g \mathbf{S}^g \dot{\gamma}^g \end{aligned} \quad (2)$$

where \mathbf{R}^h and \mathbf{S}^h are, respectively, the symmetric and skew-symmetric part of the Schmid tensor associated with the given slip system h .

For a plastic behavior, the definition of the plastic yield or critical shear stress leads to the following flow rule for a given slip system g :

$$\begin{cases} \tau^g < \tau_c^g \Rightarrow \dot{\gamma}^g = 0 \\ \tau^g = \tau_c^g \text{ and } \dot{\tau}^g \leq 0 \Rightarrow \dot{\gamma}^g = 0 \\ \tau^g = \tau_c^g \text{ and } \dot{\tau}^g > 0 \Rightarrow \dot{\gamma}^g \geq 0 \end{cases} \quad (3)$$

where τ^g and τ_c^g are, respectively, the resolved shear stress acting on the slip system g and the corresponding critical shear stress. In the present work, a new approach to determine the slip system activity in the elastic-plastic context is proposed in order to considerably reduce the computing time [8,9]. The relation linking the slip rate $\dot{\gamma}$ to the resolved shear stress rate $\dot{\tau}$ is written as $\dot{\gamma}^g = k^g (\tau^g, \tau_c^g, \dot{\tau}^g) \dot{\tau}^g$ where:

$$k^g = \frac{1}{H} \frac{1}{2} \left(1 + \tanh \left(k_0 \frac{\tau^g}{\tau_{ref}} \right) \right) \frac{1}{2} \left(1 + \tanh \left(k_1 \left(\frac{\tau^g}{\tau_c^g} - 1 \right) \right) \right) \frac{1}{2} \left(1 + \tanh \left(k_2 \frac{\dot{\tau}^g}{\dot{\tau}_{ref}} \right) \right) \quad (4)$$

H is a hardening parameter, k_0 , k_1 , k_2 , τ_{ref} and $\dot{\tau}_{ref}$ are purely numerical parameters allowing the elastic-plastic transition on a given slip system g to be followed with maximum accuracy (the reference constants τ_{ref} and $\dot{\tau}_{ref}$ only serve to make the parameters k_i dimensionless), and ‘tanh’ stands for the hyperbolic tangent function. In the above regularization function, the choice of optimal values for the numerical parameters has been motivated by a balanced compromise between accuracy and computational efficiency.

Plastic slip on a given slip system g leads generally to hardening on all the slip systems, what can be expressed by the relationship between the rate of the critical resolved shear stress acting on the considered slip system g and the total slip rate of all the active slip systems:

$$\dot{\tau}_c^g = \sum_{h=1}^{nslip} H^{gh} \dot{\gamma}^h \dot{\tau}_c^g = \frac{1}{2} \frac{\alpha \mu b}{\sqrt{\sum_{k=1}^{nslip} a^{gk} \rho^k}} \sum_{h=1}^{nslip} a^{gh} \dot{\rho}^h \quad (5)$$

The hardening matrix is expressed as a function of the mean free path

$\frac{1}{L^g} = \frac{1}{D_{moy}} + \frac{\sqrt{\sum_{h=1, h \neq g}^{nslip} \rho^h}}{g_0}$, in which D_{moy} is the average grain size and g_0 a parameter related to the storage of dislocations, the critical annihilation distance y_c and dislocation densities ρ^h of all the slip systems h . a^{gh} represents the anisotropy interaction matrix, α the dislocation interaction parameter and μ the shear modulus.

Combining the previous equations with the relationship between the nominal stress rate $\dot{\mathbf{n}}$ and the Cauchy stress rate $\dot{\boldsymbol{\sigma}}$, the local elastic-plastic tangent modulus is obtained as:

$$l_{ijkl} = \left[C_{ijkl} - \frac{1}{2} (\delta_{ik} \sigma_{lj} + \delta_{il} \sigma_{kj}) - \frac{1}{2} (\sigma_{ik} \delta_{lj} - \sigma_{il} \delta_{jk}) \right] - \left[(C_{ijpq} R_{pq}^g + S_{ip}^g \sigma_{pj} - \sigma_{ip} S_{pj}^g) M^{gh} k^h R_{mn}^h (C_{mnkl} - \sigma_{mn} \delta_{kl}) \right] \quad (6)$$

This tangent modulus is composed of elastic and plastic parts, where several convective terms appear due to the large strain framework.

2.2. Simulation of the behavior of multiphase steels

In order to deduce the overall macroscopic polycrystalline behavior starting from knowledge of the behavior of individual grains, the self-consistent scheme in the sense of Hill [10] is adopted. All the details are developed in [7,9].

In this section, the results obtained with the proposed model are compared to experimental ones (see Fig. 1). Several sequential rheological tests have been performed for a single-phase ferritic steel (IF-Ti) and a ferritic-martensitic dual-phase steel (DP). The identified parameters for these two steels are reported in Table 1 below. It is important to note that the hardening parameters, in the case of the dual-phase steel, have been taken identically for the two phases, except for the initial critical shear stress τ_{c0} and the average grain size D_{moy} , to identify the macroscopic behavior. This choice is made because the strain hardening modes in martensite are not well-known and this reduces the number of parameters that need to be identified.

| Parameter | D_{moy} (m) | τ_{c0} (MPa) | y_c (nm) | g_0 |
|-----------------------------|---------------------|-------------------|------------|-------|
| IF-Ti steel | 20×10^{-6} | 45 | 3.25 | 90 |
| DP steel: Ferritic phase | 10×10^{-6} | 180 | 2.4 | 120 |
| DP steel: Martensitic phase | 1×10^{-6} | 550 | 2.4 | 120 |

Tab. 1. Identified parameters for the two steels

As observed in Fig. 1, the numerical results obtained with the multiscale model are in agreement with experimental ones for the two steels. However, some gaps appear especially at the onset of the plastic regime during the second loading path for Bauschinger tests and orthogonal test. These gaps increase as pre-strain gets larger. They can be explained by the fact that the spatial rearrangement of dislocation cells is not taken into account in the present model. Experimental evidence of such a rearrangement can be found easily in the literature for IF-steels [11]. In the present model, the internal variable acting at this scale is the mean dislocation density for a slip system. At the onset of the second loading path, the structure of the dislocation cells is disintegrated and another one depending on the

second loading path is created [12], which may explain the observed differences. In order to reduce this gap an idea would consist in introducing kinematic hardening at the slip system level (the kinematic hardening in the present model is only inter-granular and not intra-granular due to the self-consistent scheme) [13,14]. The DP steel presents the same previously observations as the single phase steel ones. However, the agreement of the model with experimental data during sequential loadings is better due to the less-pronounced effect of dislocation cells for this material in comparison with the first one. On the whole, the proposed multiscale model is able to reproduce the elastic-plastic behavior of single as well as dual phase polycrystalline materials.

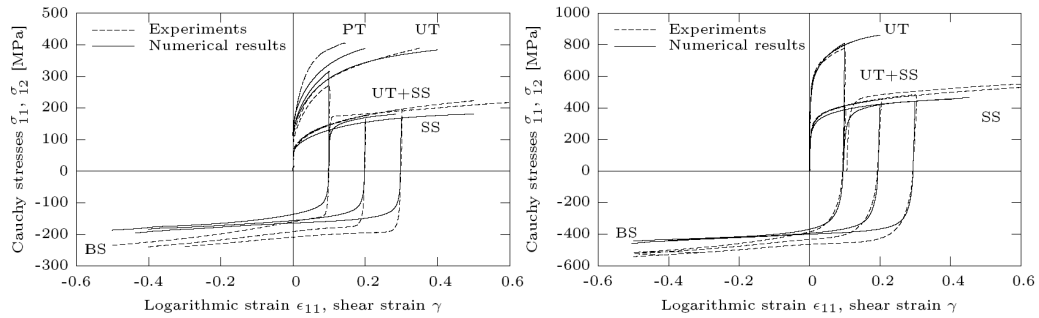


Fig. 1. Comparison model/experiments of the stress-strain behavior during different strain paths performed perpendicular to RD (PT for Plane Tension, UT for Uniaxial Tension, SS for Simple Shear, BS for Bauschinger Shear and UT+SS for cross test) for an IF-Ti steel (at left) and for a Dual Phase steel (at right)

3. Ductility loss modeling

3.1. Strain localization criterion – Rudnicki-Rice model

The so-called Rudnicki-Rice criterion [1,2] corresponds to a bifurcation associated with admissible jumps for strain and stress rates across a shear band as illustrated in Fig. 2.

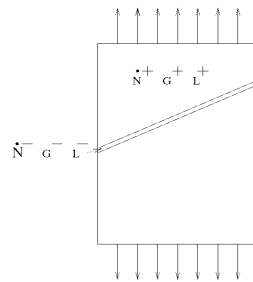


Fig. 2. Localization of the deformation along a shear band

Since field equations have to be satisfied, and because the strain rate is discontinuous across the localization band, a kinematic condition for the strain rate jump must be verified. On the other hand, the continuity of the stress rate

vector has to be verified for the forces along the interface created by the localization band (see [9] for more details).

Combining all these conditions, the ductility loss criterion can be easily expressed as a function of the only macroscopic elastic-plastic tangent modulus by:

$$\det(\mathbf{v} \cdot \mathbf{L} \cdot \mathbf{v}) = 0 \quad (7)$$

In the above condition, corresponding to the singularity of the acoustic tensor and associated with loss of ellipticity of field equations, \mathbf{v} is the unit normal to the shear band.

3.2. Prediction of Forming Limit Diagrams of multiphase steels

In this part, direct FLDs simulated for the two steels studied in the previous part are compared to the FLDs provided by ArcelorMittal. The FLDs from ArcelorMittal were obtained using a model developed by Cayssials [15,16]. This model, commonly used by ArcelorMittal, has proven to be reliable in predicting formability for linear loading paths. In particular, the validity of this ArcelorMittal's FLD model has been assessed through a wide range of grades of sheet metals, for which experimental FLDs have been simultaneously measured. Despite its good results, its restriction to linear loading paths together with its phenomenological basis, in which microstructural effects cannot be accounted for, have motivated the development of the proposed approach with the aim of designing new materials. The results given by the proposed model based on Rice's localization criterion are reported in Fig. 3.

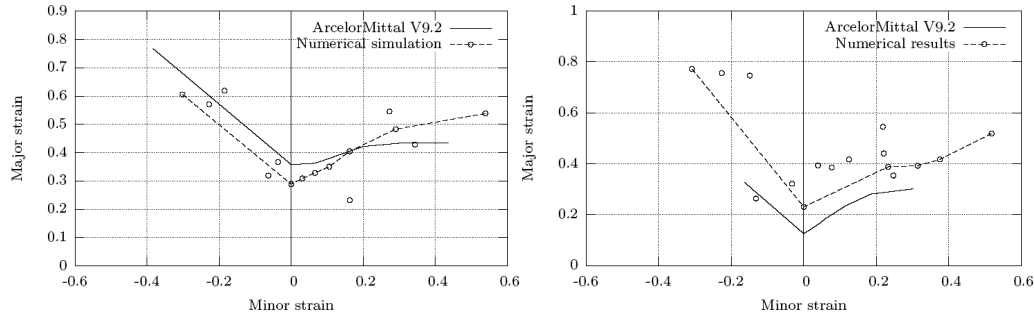


Fig. 3. Comparison between direct simulated FLDs and ArcelorMittal's reference FLDs for an IF-Ti steel (at left) and for a DP steel (at right)

The simulated FLDs for the two steels are close to the ArcelorMittal's ones. Although the FLD for the IF-Ti steel seems to be a little underestimated and that for the DP steel is overestimated, the impact of the metallurgy on the formability is correctly reproduced since the addition of a hardening phase such as the martensite leads to a decrease in ductility in comparison to the single-phase steel. As it can be also seen in Fig. 3, some localization points, given by the model, exhibit certain dispersion in the expansion domain.

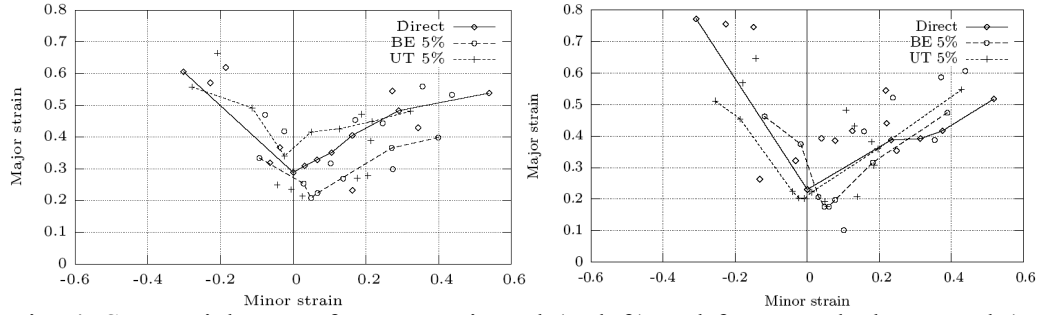


Fig. 4. Sequential FLDs for an IF-Ti steel (at left) and for a Dual Phase steel (at right)

In Fig. 4, FLDs are plotted with two different pre-strains for the two steels. Only a qualitative comparison can be made since no experimental or reference results are available, as ArcelorMittal's FLD model is not designed to predict formability when two-stage or more complex loading paths are considered. Nevertheless, Haddad [17] has shown that during a second loading path, the FLD is shifted in the direction of the first path. For example, in the case of uniaxial tension pre-strain the curve is expected to be translated along the preloading direction. This is clearly found with the present model.

3.3. Impact of physical parameters on ductility limit

It is also interesting to investigate the impact of microstructural mechanisms on ductility, which can be advantageously used in the design of new materials in order to optimize their formability and mechanical properties in-use. The effect of the four physical parameters of the multiscale model on the three extreme points (uniaxial tension, plane tension and equibiaxial expansion) of the FLD has been analyzed and the results are shown in Fig. 5 and Fig. 6.

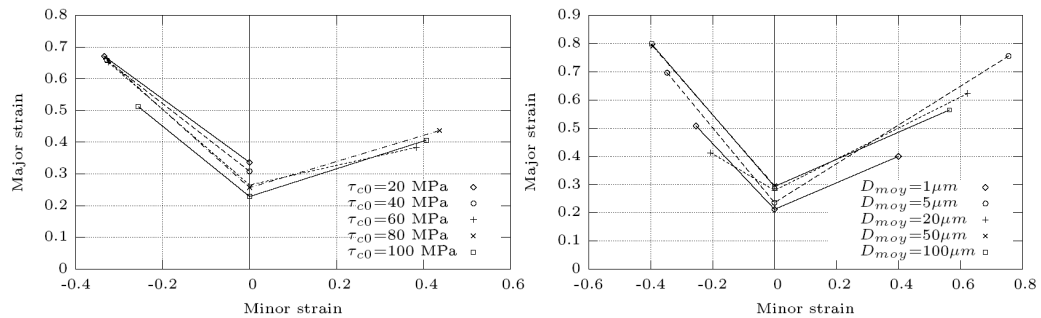


Fig. 5. Effect of the initial critical resolved shear stress τ_{c0} (at left) and of the average grain size D_{moy} (at right) on direct FLDs for an IF-Ti steel

As depicted in Fig. 5, a decrease of the initial critical resolved shear stress τ_{c0} leads to an improvement of the ductility. This result can be compared to the Luft work [18] reporting that a decrease of the temperature during uniaxial tension on single crystals of molybdenum resulted in an increase of the elastic limit and thus

a decrease of ductility. The initial critical resolved shear stress τ_{c0} being linked to the elastic limit during uniaxial tensile test, the effects found by the proposed model is in agreement with Luft's ones.

It is also known that a decrease of average grain size produces higher-strength materials but, in turn, induces a drop in ductility. This experimental observation is found by the model as shown in Fig. 5.

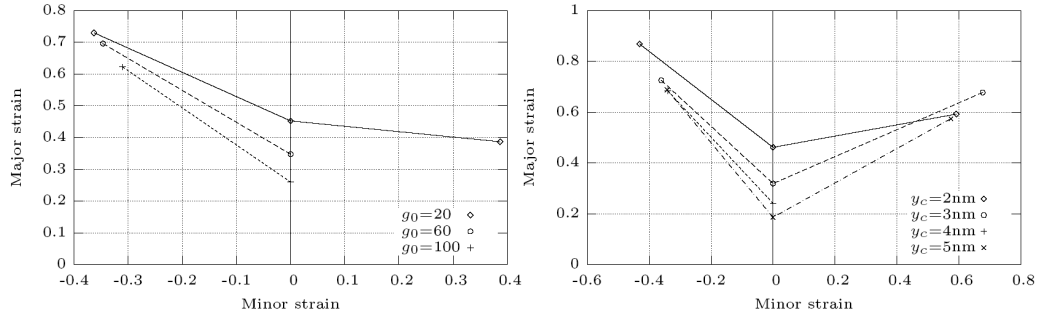


Fig. 6. Effect of the storage parameter g_0 (at left) and of the critical annihilation distance y_c (at right) on direct FLDs for an IF-Ti steel

Fig. 6. reveals that the ductility of the single-phase steel will improve with lower values for parameter g_0 . It means that a higher mean free path of dislocations will deteriorate the formability. In the same way, an important critical annihilation distance y_c will limit the steel ductility. This effect is well reproduced by the model as depicted in Fig. 6.

4. Conclusions

In this paper, a multiscale model has been combined with Rice's criterion in order to analyze the formability of multiphase steels in sheet forming processes. Numerical FLDs have been plotted and compared to reference ones. To do that, the macroscopic behavior law has been accurately modeled in order to take into account the most important softening mechanisms so that the effects of complex loading paths are at least partially captured. The introduced ductility criterion allows the determination of FLDs which are close to reference FLDs and reproduces qualitatively the effects of complex loading paths.

This theoretical and numerical tool allows the ductility prediction of new materials from the early stage of the design of new grades of steel and thus provides a useful tool for steelmakers like ArcelorMittal. Its main interest is to allow comparisons in terms of formability of those materials and to determine the impact of microstructural effects on the ductility. Therefore, it can be advantageously used to optimize the ductility of new steels or to design materials with desired formability.

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