

Description of microstructural intragranular heterogeneities in a Ti-IF steel using a micromechanical approach

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Abstract. A classical problem in metallurgical research is to control the recrystallisation texture which forms during the last annealing process and which determine the mechanical behaviour of the final products. It is now widely admitted that the local deformed state and the substructural heterogeneities within the polycrystal are key parameters to understand the recrystallisation mechanisms.

In this work, we present a micromechanical approach based on the use of the affine extension of the self-consistent scheme for viscoplastic behaviours and a phenomenological description of dislocation patterning using a hardening model recently developed for two-stage strain paths. These two ingredients allow to compare the model with experimental crystallographic texture after rolling as well as experimental observations of the intragranular substructure using orientation imaging by Electron Back-Scattered Diffraction. It is shown that the rolling texture is correctly simulated and successful predictions of the orientation of dislocation sheets are obtained.

1. INTRODUCTION

To create the desirable crystallographic textures that improve the formability properties of low carbon steels, a high degree of deformation by cold-rolling is needed. Since it is evident that this deformation substructure plays an important role in the nucleation process during recrystallisation (see e. g. [1]), it is important to characterize deformation heterogeneities and to explore the possibilities to link them with a micromechanical model describing the deformation process. We present here a micromechanical approach based on the use of the affine extension of the self-consistent scheme. A local hardening law based on dislocation patterning is used to describe the evolution of the dislocation density within the walls. In this paper, we report results obtained in the characterization of the deformation traces often observed in several grains after etching in a cold-rolled IF steel. The deformation traces are first analysed from EBSD scans in relation with their crystallographic orientation and then compared to cell-block boundaries (CBBs) predicted by the micromechanical model.

2. EXPERIMENTAL PROCEDURE

2.1. Material studied

The material studied is a Ti-IF steel, issued from a previous hot rolling, which presents an average grain size of $20\mu\text{m}$ and a low crystallographic texture (Figure 1). It has been deformed by cold-rolling with different thickness reductions (15%, 30%, 40% and 50%) in a laboratory rolling mill. The crystallographic texture of the material after cold-rolling presents classically two fibers : α ($\langle 110 \rangle$ direction aligned with the rolling direction) and γ ($\{111\}$ pole aligned with the normal direction of the sheet). The maximum value of the orientation distribution function (ODF) is located in the α fiber.

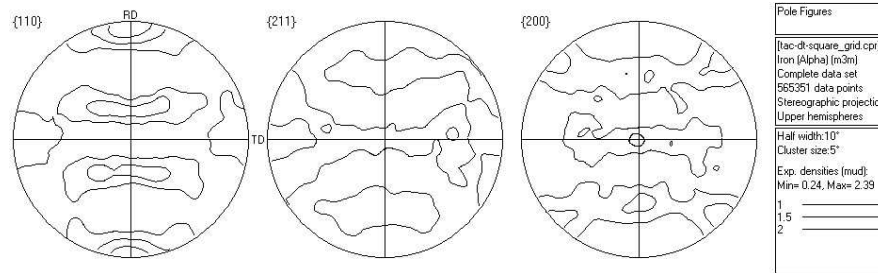


FIGURE 1. Pole figures of the Ti-IF steel in the as-received state (hot band)

2.2. Experimental analysis of the substructure

The dislocations tend to form structures during plastic deformation. It is well established that the morphology of the structure depends on numerous parameters : the number of active slip systems, the grain size, the crystalline structure . . . In our case, a cellular structure with dislocation sheets parallel to the crystallographic planes of highest plastic slip activity is expected [2]. The development of such structures, implying significant intragranular misorientations, can be studied using (i) the orientation imaging technique based on electron back-scattered diffraction (EBSD) within a scanning electron microscope (SEM) and (ii) “direct” observations of the local strain field caused by dislocations by transmission electronic microscopy (TEM).

EBSD measurements were carried out on a Cambridge S360 with an operating voltage of 25kV and a probe current of about 3nA. All observations were made on the section normal to the transverse direction (TD) with a step size of 200nm. The samples were mechanically polished and then electro-polished to remove any work-hardened surface layer with a solution made up of 5% of perchloric acid and 95% of ethanol during 10s at 38V. The inclination of the traces along the rolling direction is regarded versus their orientation or, more exactly, the orientation just near that trace inside the considered grain. For example, in figure 2 we can see two areas (delimited by white ellipsoids) inside the same grain with several parallel traces. In this case only one orientation and one inclination for this set of traces are noted.

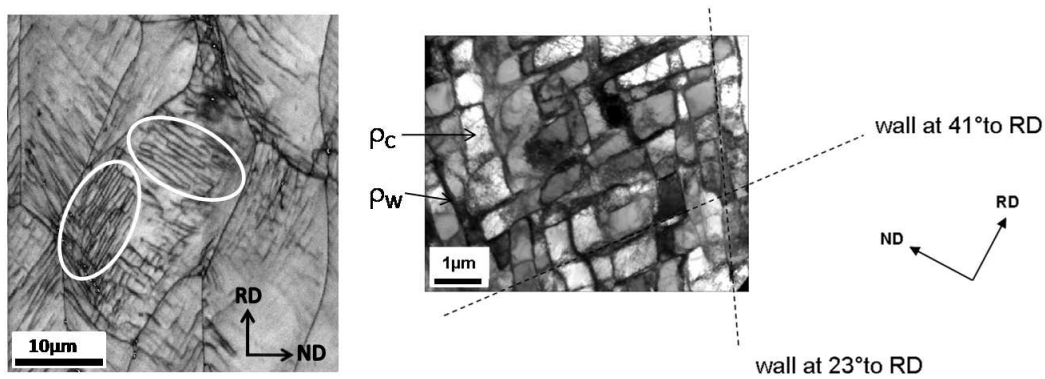


FIGURE 2. Image quality EBSD map after 30% of thickness reduction (step size of 0.1µm) and TEM micrograph in bright field showing dislocation microstructure after 40% of thickness reduction

Their main inclination can be compared to the dislocation walls observed with TEM in these materials. For instance, for a sample cold-rolled up to 40% thickness reduction, the mean trace inclination along RD is about 38° (average value obtained for a set of 20 grains) and in TEM we generally observed 2 dislocation walls.

3. MICROMECHANICAL MODELLING

3.1. Transition-scale scheme

To predict the local and overall response of the Ti-IF steel, we adopt a micromechanical approach which allows to derive the mechanical behaviour and the microstructural evolution (especially the development of crystallographic texture) of the polycrystal from the behaviour of the constituent grains. In this framework, a polycrystal is viewed as a composite material with a large number of mechanical phases and a granular topology. A phase includes all the grains with the same crystalline orientation. The homogenisation procedure delivers an estimation of the macroscopic response and a statistical description of the stress and strain fields within each phase (average, standard deviation etc ...) by making use of Eshelby's inclusion formalism. For polycrystalline microstructures, it is known that the most relevant model is the self-consistent scheme which assumes that each phase plays the same role from a morphological point of view (concept of perfect disorder [3]).

For plastic behaviours, and more generally for any nonlinear constitutive laws, an additional choice has to be made regarding the way the nonlinear response can be obtained from a classical linear homogenisation model. Here, we adopt the so-called affine extension of the self-consistent scheme. It has been shown [4, 5] that this affine approach leads to a more realistic description of the (visco)plastic behaviour than the usual secant model of Hill and Hutchinson [6, 7]. Besides, it presents interesting connections with some more advanced variational formulations [8].

3.2. Constitutive viscoplastic flow rule

It is assumed that the deformation occurs by viscoplastic glide on the following slip systems : $\langle 111 \rangle \{1\bar{1}0\}$ and $\langle 111 \rangle \{11\bar{2}\}$. On a slip system k , the flow rule reads

$$\dot{\gamma}_k = \dot{\gamma}_0 \left| \frac{\tau_k}{\tau_0^k} \right|^{n-1} \frac{\tau_k}{\tau_0^k}, \quad (1)$$

with τ_k the resolved shear stress, $\dot{\gamma}_k$ the slip rate and τ_0^k the reference (critical) shear stress. To describe the plastic behaviour of steel at room temperature, we consider a nonlinear exponent $n = 40$ and a reference slip rate $\dot{\gamma}_0 = 10^{-11} \text{s}^{-1}$ [9]. Finally, it is necessary to specify the value of the reference shear stress τ_0^k and its evolution with the deformation.

3.3. Local hardening law based on dislocation patterning

To take into account phenomenologically the dislocation patterning, Peeters *et al.* [10] proposed a local hardening law which makes use of dislocation densities. Compared to previous approaches like the one developed by Tabourot *et al.* [11], this model supposes that cell-block boundaries form during deformation. It is assumed that these dislocation sheets form parallel to (110) crystallographic planes. To describe this structure, use is made of different variables : the dislocation density ρ_c within the cells, the dislocation density ρ_w within the walls (dislocation sheets) and a ‘‘polarized’’ dislocation density ρ_p . Each of these variables has its own evolution equation which follows the general form $\dot{\rho} = (A\sqrt{\rho} - B\rho)|\dot{\gamma}|$. This leads to a stationary state with a saturation of the dislocation densities. For more details, the reader is referred to [10].

The following features can be pointed out :

- At each time step, the model assumes that cell-block boundaries form on the two (110) planes of highest slip activity.
- During a strain-path change, progressive destruction of old CBBs occurs. This feature must be considered even in the present case of a radial and monotonic loading because of the crystalline rotation which implies a continuous strain-path change for each orientation. Consequently, it is worth noting that more than two CBBs can exist within a crystalline orientation.
- The CBBs are associated with latent hardening since they act as obstacles for the mobile dislocations on subsequently activated slip systems.
- The reference shear stress τ_0 is obtained by a rule of mixture within each crystalline orientation according to the ‘‘composite’’ model of Mughrabi [12]. It reads

$$\tau_0 = (1 - f_w)\tau^C + f_w \sum_{i=1}^6 \tau_i^{\text{CBB}} \quad (2)$$

with f_w the volumic fraction of CBB, τ^C the reference shear stress within the cells and τ_i^{CBB} the reference shear stress for each potential cell-block boundary.

The parameters identified in [10] have been used. They lead to a saturating dislocation density of $1.3 \cdot 10^{-15} \text{m}^{-2}$ within the CBBs. A nice feature of this model is that it allows to link intragranular crystalline misorientations with a specific dislocation density ρ_w .

4. RESULTS AND DISCUSSION

The model has been used to simulate (i) the overall response, including the crystallographic texture evolution and (ii) the dislocation patterning at the intragranular level. Simulations are performed up to 50% of thickness reduction. Concerning the microstructural description of the initial state of the polycrystal, it must be noted that the crystallographic texture of the hot-band (Figure 1) is used and that a random distribution of equiaxed grain is assumed.

The model is able to capture the intergranular heterogeneity within the polycrystal. Indeed, it predicts a higher mean deformation for the grains belonging to the α fiber compared to the mean deformation within the γ fiber. Concerning the overall crystallographic texture, a rather good description of the main texture components is obtained (Figure 3). Especially, compared to Taylor-like models, the γ fiber is correctly predicted. Nevertheless, it can be observed that the intensity of this fiber is too high with respect to the experimental texture.

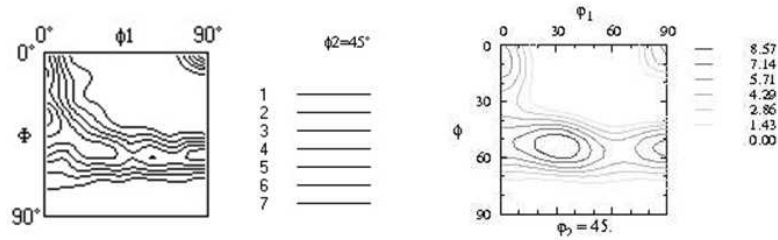


FIGURE 3. Experimental versus simulated ODF obtained with the affine self-consistent model (50% thickness reduction)

To compare experimental traces with CBBs predicted by the model, we considered different initial crystallographic textures : isotropic texture described by a set of 2016 orientations following the vector method and two sets of orientations randomly taken from an EBSD scan of the as-received state (respectively 1000 and 3000 points). For the experimental crystallographic texture, it has been checked that the ODF obtained with the two sets is comparable to the one obtained with the entire EBSD scan.

From EBSD observations, we know the orientation of the grain (\mathbf{g}_{exp}) near each experimental trace and for each strain level observed. From the modeling, for each deformation step, we have a new set of orientations and we extract the ones at less than 5° from \mathbf{g}_{exp} . Then, we have access to the dislocation density and the inclination along the rolling direction for each dislocation walls for a set of orientations near experimental ones. We then compare the inclinations of the two predicted walls with maximum dislocation densities, for all orientations at less than 5° from \mathbf{g}_{exp} , with the inclination of the experimental trace. It is worth noting that the model often predicts only two dislocations walls with a high dislocation density for a given crystalline orientation.

Besides, we mention that within the set of crystalline orientations predicted by the micromechanical model, it is possible to have grains with close crystalline orientations but different deformation histories because of the texture evolution and work-hardening.

Our analysis shows that there is a correct agreement between experimental traces and predicted CBBs. Besides, the best agreement is obtained when considering the real initial texture represented by 3000 orientations (Table 1). Interestingly, it has to be noted that the majority of experimental traces that do not correspond to the CBBs predicted by the model belong to grains with a high orientation gradient. This observation might be related with the fact that the self-consistent model only consider average orientations per phase. It could also be necessary to consider the formation of CBBs on (112) planes in the hardening model.

TABLE 1. Agreement between experimental traces and predicted CBBs.

Isotropic	Exp. ODF (1000 points)	Exp. ODF (3000 points)
60% \pm 12%	57% \pm 9%	66% \pm 7%

5. CONCLUSIONS

By comparing experimental with simulation results we show that the evolution of the deformation substructure of this Ti-IF steel is quite well reproduced by the present model with a good prediction of dislocations sheets up to 50% cold-rolling. Since the deformation texture is also well estimated, we now aim at coupling these results with a recrystallisation model to predict the kinetic of subsequent static recrystallisation and the final crystallographic texture. For that goal, the possibility of considering specific dislocations densities, linked to interior cells and cell-block boundaries, is very attractive to describe phenomenologically the so-called grain fragmentation and its influence on recrystallisation.

REFERENCES

1. M. R. Barnett, *ISIJ Int.* **38**, 78–85 (1998).
2. B. Peeters, B. Bacroix, C. Teodosiu, P. van Houtte, and E. Aernoudt, *Acta Mat.* **49**, 1621–1632 (2001).
3. E. Kröner, *J. Mech. Phys. Solids* **25**, 137–156 (1977).
4. R. Masson, and A. Zaoui, *J. Mech. Phys. Solids* **47**, 1543–1568 (1999).
5. R. Brenner, O. Castelnau, and L. Badea, *Proc. R. Soc. Lond.* **A460**, 3589–3612 (2004).
6. J. W. Hutchinson, *Proc. R. Soc. Lond.* **A319**, 247–272 (1970).
7. J. W. Hutchinson, *Proc. R. Soc. Lond.* **A348**, 101–127 (1976).
8. R. Masson, M. Bornert, P. Suquet, and A. Zaoui, *J. Mech. Phys. Solids* **48**, 1203–1226 (2000).
9. P. Eriean, Ph.D. thesis, Ecole Centrale Paris (2003).
10. B. Peeters, M. Seefeldt, C. Teodosiu, S. R. Kalidindi, P. van Houtte, and E. Aernoudt, *Acta Mat.* **49**, 1607–1619 (2001).
11. L. Tabourot, M. Fivel, and E. Rauch, *Mater. Sci. Engin.* **A234-236**, 639–642 (1997).
12. H. Mughrabi, *Mater. Sci. Engin.* **85**, 15–31 (1987).