

Modeling of microscopic strain heterogeneity during wire drawing of pearlite

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Abstract

An original strategy is proposed in order to perform computationally affordable, direct micro-to-macro simulations of metal forming operations. The model is implemented as a user-defined material law in the abaqus finite element code. This allows accounting for the evolving microstructure in both single and multiphase metallic alloys undergoing large plastic deformation. The model is used here to predict strength and texture development in pearlitic steel. At the scale of individual lamellae, stress equilibrium is enforced across cementite-ferrite interfaces and plasticity is achieved by dislocation glide. Three hypotheses are tested about the interaction of adjacent colonies, including a simplified - so called “multisite”- modeling of the stress and strain partitioning on either sides of planar grain boundary segments. The latter approach gives rise to a slower and more realistic prediction of the texture development and the progressive alignment of cementite lamellae with the loading axis.

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1. Introduction

Modern multiphase metallic alloys often demonstrate increased strength and toughness as a result of the microstructural changes occurring during metal forming operations. Successful manufacturing of high strength multiphase alloys requires proper understanding of the build up of very large internal stresses and anisotropy. Micromechanical models can assist technological developments on the condition that they allow computationally affordable prediction of the polycrystal plastic deformation during real-scale simulation of forming processes.

Over the years, several theoretical models (e.g. [1-4]) have considered wire drawn pearlitic steel in which the microstructure consists of a thin stacking of ferrite and cementite. The extremely strong cementite lamellae are only a few nanometers thick. The strength of the softer ferrite depends on the inter-lamellar spacing. Both phases contribute to a composite mechanical response, which is anisotropic due to crystallographic texture [5] and to the progressive preferential alignment of cementite lamellae according to the loading directions [6]. It has been observed that microcracking during forming may result from excessive internal stresses due to the huge strength contrast between the two phases [7-9].

The crystal plasticity model used in the present study predicts the dislocation slip activity within individual grains and the resulting rotations of the crystal lattices. Its main originality is the simplified treatment of the interaction of adjacent crystallites, which accounts for the distribution of grain shapes and sizes. The model was so far mostly applied

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to single phase metals, leading to improved predictions of the developed crystallographic texture [10] and the induced plastic anisotropy [11]. The numerical implementation of the model as a user-defined material law (UMAT) in the abaqus finite element code has enabled performing direct micro-to-macro modeling of deep drawing of steel sheets using either 3D elements [12] or shell elements [13].

Extension of the latter model from single to multiphase polycrystalline materials is rather straightforward as explained in Section 2. Whereas it has sometimes been assumed that the thin stacking of ferrite and cementite lamellae imposes uniform deformation of the two phases [1-3], it is demonstrated in Section 3 that testing other hypotheses about the compatible co-deformation of the dual-phase aggregate influences the composite response and the developing texture.

2. Model description

2.1. Dislocation mediated plasticity inside ferrite and cementite

The crystal plasticity model is described in detail elsewhere [10,13,14]. The multiplicative decomposition of the deformation gradient tensor involves a rotation of the crystal lattice, an infinitesimal elastic stretch and a plastic deformation that is due to dislocation slip only. In the case of pearlitic steel, dislocations glide along $\{110\}\langle 111 \rangle$ and $\{112\}\langle 111 \rangle$ systems in ferrite, whereas $(010)[001]$ and $(110)[\bar{1}\bar{1}1]$ slip systems operate in cementite which has orthorhombic symmetry ($a = 5.0816 \text{ \AA}$, $b = 6.7446 \text{ \AA}$, $c = 4.5206 \text{ \AA}$).

For simplicity, both phases are here assumed to undergo isotropic strain hardening. If Γ denotes the total slip on all slip systems, the critical resolved shear stress follows an exponentially saturating law (Voce). τ_c thus increases from the initial value τ_{c0} to the maximum value τ_{sat} whereas Γ_0 scales with the initial hardening:

$$\tau_c = \tau_{sat} - (\tau_{sat} - \tau_{c0}) \exp(\Gamma/\Gamma_0). \quad (1)$$

The values of all material parameters used in the present study have been determined by fitting uniaxial tensile test measurements performed before and after rolling of pearlitic steel sheets [15]. Using the set of parameters listed in Table 1, the model reproduced elastic lattice strains measured by neutron diffraction [14]. However, hardening of ferrite is not related directly to the thinning of interlamellar channels.

Table 1. Fitted material parameter values

	τ_{c0} [MPa]	τ_{sat} [MPa]	Γ_0
Ferrite	250	380	65
Cementite	1600	2000	10

2.2. Strain heterogeneity among adjacent crystallites

The two-scale modeling scheme is depicted in Figure 1. The deformation of every crystallite corresponds to the superposition of a homogeneous strain applied to the pearlite colony hosting the crystallite and a strain relaxation allowing cementite and ferrite lamellae to undergo different (geometrically compatible) strains.

Inside every colony, successive lamellae undergo opposite shear strain parallel to the cementite-ferrite interface as well as heterogeneous strain normal to the interface. The amplitude of such strain relaxation is computed in such a way that stresses are balanced across the ferrite-cementite interfaces, which also corresponds to a minimum of the average plastic dissipation energy. Superimposed to the latter deformation, the colony undergoes a uniform strain, which may differ from the macroscopic strain as a result of its interaction with surrounding colonies. Three modeling hypotheses are tested here:

- According to the “full constraints” version of the model, all colonies undergo the same average strain, which is equal to the macroscopic strain.

- According to the “relaxed constraints” version of the model, individual colonies can deform freely in the plane perpendicular to the macroscopic tensile direction (termed “longitudinal direction” in the sequel). Colonies are also free to shear along the latter direction. This means that the average stress of every colony is uniaxial, and the macroscopic strain is achieved only on average over the whole (randomly oriented) polycrystal.
- The third version of the model is called multisite. It is inspired from the ALAMEL texture prediction model [10]. Pairs of adjacent colonies interact across a planar grain boundary (right of Fig. 1) and stress equilibrium is enforced across such boundary. The induced local strain heterogeneity warrants that the macroscopic strain is achieved on average over every pair of interacting colonies.

In reality, pearlite colonies are observed to undergo fragmentation after large strains. This phenomenon is not considered here but it could be investigated by relying on a finite element model (instead of the three simplified hypotheses listed above) in order to simulate the interaction of adjacent colonies.

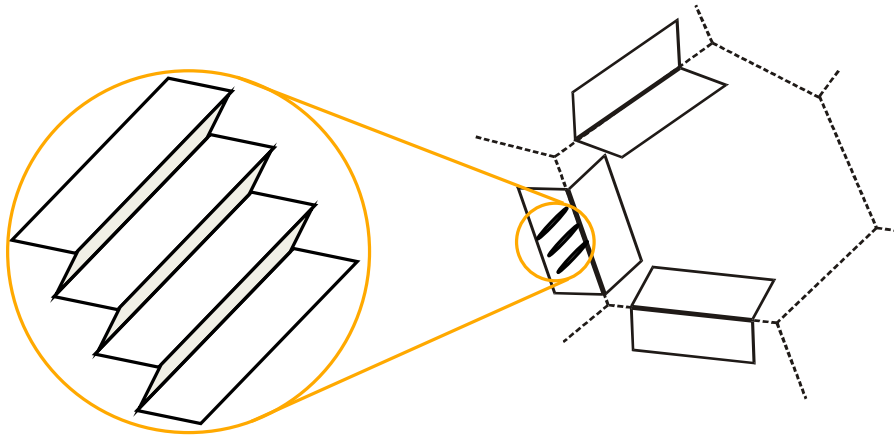


Fig. 1. Illustration of strain heterogeneity occurring at two levels: between adjacent pearlite colonies when relying on the multisite model (right) and inside each colony (left) due to stacking of soft ferrite and hard cementite lamellae.

2.3. Micro to macro scale transition

The macroscopic stress is computed as the average stress within a representative volume element reproducing the local crystallographic texture and the distribution of grain shapes and of orientations of ferrite-cementite interfaces in the evolving microstructure.

When the model is used as a user-defined material law in real-scale simulation of forming operations, the computational cost is reduced by relying on locally incomplete orientation samplings [12-13]. A different set of lattice orientations is assigned to every integration point and it is ensured that both the overall texture and the orientations of ferrite-cementite stacking are statistically reproduced over about 10 adjacent finite elements.

In the present study, the focus is set on the comparison of the three alternative modeling hypotheses about the interaction of adjacent colonies (Section 2.2). The stand-alone version of the model is used because the relaxed constraints version does not allow computing a consistent tangent operator as required by the iterative solver of a macroscopic finite element simulation. The history of deformation experienced by the material during wire drawing is computed in a preliminary simulation relying on isotropic J_2 plasticity and the crystal plasticity model is used in post-processing.

3. Results

3.1. Simulation of a uniaxial tensile test

As a preliminary investigation, the pearlitic steel is considered isotropic. It is made of a polycrystal with equi-axed grains and with a random crystallographic texture. The orientations of the pearlite lamellae are random too. The volume fraction of cementite is 12%. The representative volume element used in the simulation contains 2000 colonies, which is enough in order to predict an isotropic mechanical response with an accuracy of about 1%. For the MS version of the model, pairs of adjacent colonies are randomly selected among the sampling of 2000 colonies.

As shown in Fig. 2, the three different hypotheses about the interaction of adjacent pearlite colonies influence the prediction of the macroscopic longitudinal stress during uniaxial tension. The prediction of the multisite version of the model is intermediary between the other two. All versions of the model predict that the strong cementite deforms somewhat less than the soft ferrite. The latter result tends to indicate that the experimentally observed thinning of ferrite channels cannot be deduced directly from the macroscopic strain.

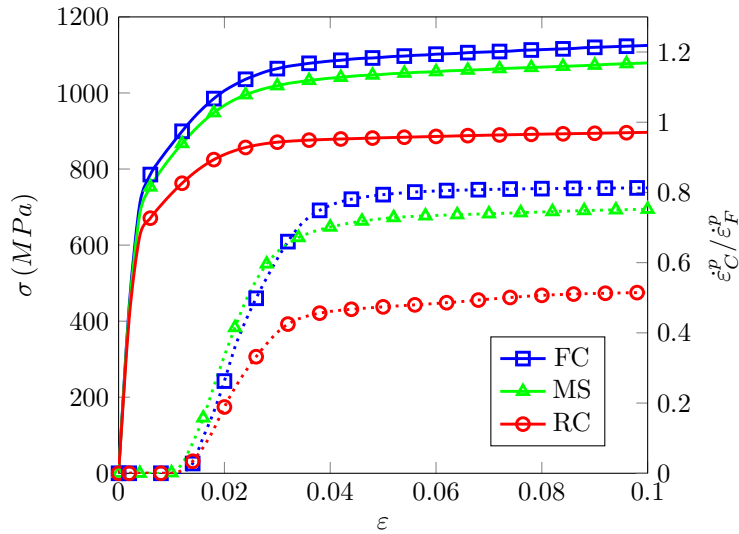


Fig. 2. Comparison of predicted uniaxial stress (continuous lines, left axis) and strain partitioning between cementite and ferrite (dotted lines, right axis) based on different assumptions about interaction of adjacent colonies.

3.2. Simulation of wire drawing

The same model polycrystal is now used as initial material in order to simulate wire drawing up to a longitudinal elongation of 740% (equivalent plastic strain of 2 along the wire axis). In Fig. 3a, the initial crystallographic texture is represented by an inverse pole figure. This means that the macroscopic longitudinal direction e_z and the radial (or transverse) direction e_r are projected in a reference system matching the cubic crystal lattice of ferrite. The uniform distribution of poles in the inverse pole figure is indicative of a random texture. The cementite lamellae were introduced by randomly selecting a variant of the Isaichev orientation relationship [15] within each grain. Hence, the interface normal is (110) in cementite and (112) in ferrite. Moreover (010) in cementite is parallel to (111) in ferrite. The prescribed crystalline orientation of the interface is shown in Fig. 3a (projection of (112) in the inverse pole figure).

There is a significant microstructural evolution during wire drawing. In the model, this is accounted for by imposing a rotation of the pearlite lamellae, which depends on the average strain of the colony and is hence different for every one of them. Fig. 3b shows the evolution of the average tilt angle of the cementite-ferrite interface normal relative to

the drawing axis $\mathbf{e}_z$. A similar rotation, but computed from the macroscopic strain, applies to the planar grain boundary separating adjacent colonies in the MS model.

The crystallographic texture predicted after wire drawing is presented in Fig. 4. It is computed for the centre of the wire where the macroscopic deformation is axi-symmetric, and also for the skin of the wire where $\mathbf{L}_{zx}$ shear is significant when passing across the die (according to the finite element simulation). Independent of the model version, ferrite crystallites tend to align (110) with $\mathbf{e}_z$. The multisite version of the model predicts a slower texture development as compared to relaxed and full constraints versions and, in terms of stable texture components, its prediction is between the other two. According to the relaxed constraints version of the model the cementite-ferrite interface tends to align with (100). There is no such preferential alignment of the lamella interface under full constraints and multisite grain interaction. According to the latter two models, the main difference between the centre and the skin of the wire is a slight tendency to align (110) with $\mathbf{e}_r$ in the skin.

4. Discussion

In Fig. 2, the distinct predictions of the three versions of the model indicate that strain heterogeneity between cementite and ferrite has a significant influence on the macroscopic strength. The greater the strain heterogeneity allowed at the level of adjacent colonies, the more significant is the partitioning of strain between the hard cementite and the soft ferrite (see also [4]). A steady state regime seems to appear after about 5% elongation. However, this no longer holds after very large strains, when lamellae are aligned with the drawing direction (Fig. 3b) reducing the strain heterogeneity (not shown).

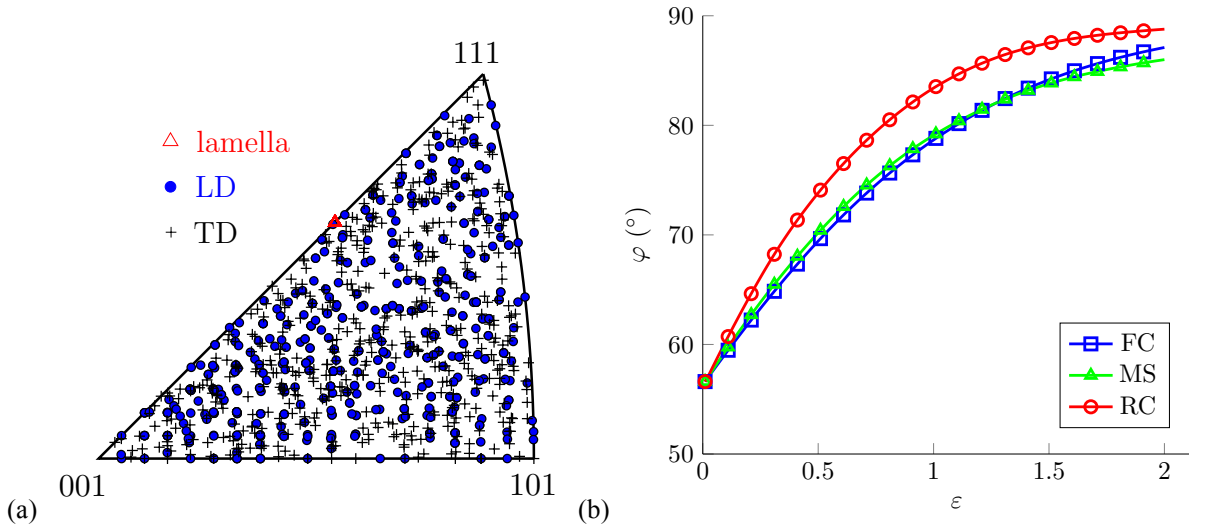


Fig. 3. (a) Inverse pole figure representing the initial alignment of the wire longitudinal axis ($\text{LD}=\mathbf{e}_z$), the transverse direction ($\text{TD}=\mathbf{e}_r$) and the lamella normal direction in a coordinate system defined along the crystal lattice of the ferrite crystallites. (b) Average tilt angle of the cementite-ferrite interface normal relative to the longitudinal axis $\mathbf{e}_z$.

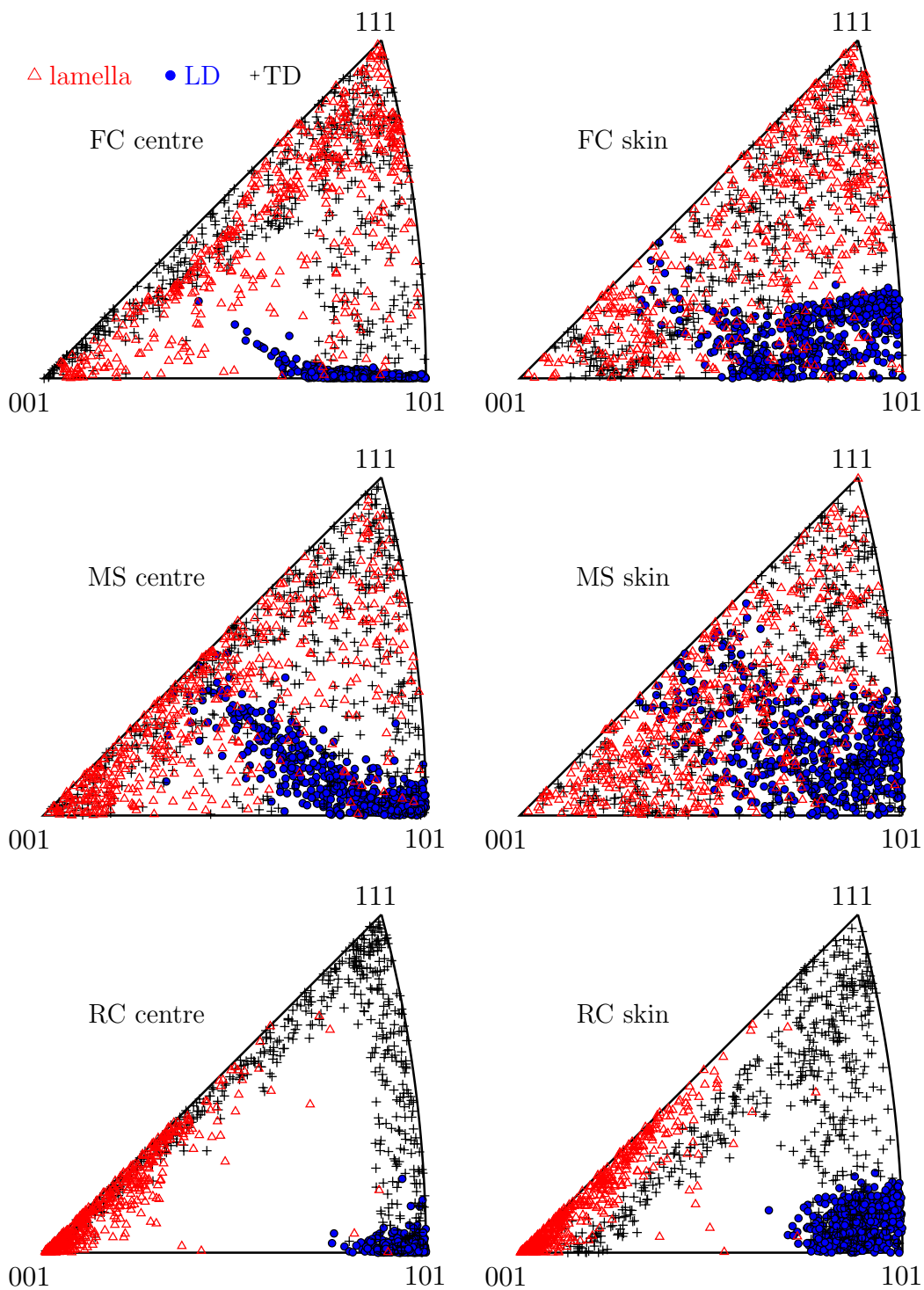


Fig. 4. Comparison of the textures predicted in the centre (left) and on the skin (right) of a pearlitic drawn wire when relying on the full constraints (FC) model (top), the multisite (MS) model (middle), and the relaxed constraints (RC) model (bottom).

The influence of the interaction between adjacent colonies is also evident in Fig. 4. The relaxed and full constraints versions of the model predict a rapid rotation of the (110) crystal direction towards the drawing axis. In experimental measurements [6,15], the texture development is slower and it conforms better to the multisite prediction. Similar observations were made after rolling of single phase metals [10]. The [110](1-10) component predicted at the skin of the wire, due to shear, has been reported in experiments [6] together with other texture components, such as [112](1-10), which the multisite model predicts but with very low intensity. The crystal orientation of the normal to the pearlite lamellae could also be used to assess the model. This is the object of ongoing research.

Conclusion

Crystal plasticity predictions have demonstrated that the macroscopic strength and the microstructural changes during wire drawing of pearlite are both influenced by the microscopic strain heterogeneity resulting from the interaction of adjacent (and differently oriented) pearlite colonies.

The proposed two-scale model produces realistic predictions of the strength and crystallographic texture development. It is computationally efficient, allowing direct micro-to-macro modeling of forming operations. The model should however be further assessed against experimental measurements of microtexture and internal stresses.

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