New mesoscopic constitutive model for deformation of pearlitic steels up to moderate strains

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Abstract. A new constitutive model for deformation of pearlitic steels has been developed that describes the mechanical behaviour and microstructural evolution of lamellar multi-colony pearlite. The model, a two-phase continuum model, considers the plastic anisotropy of ferrite derived from its lamellar structure but ignores any anisotropy associated with cementite and does not consider the crystal structure of either constituent. The resulting plastic constitutive equation takes into account a dependence on both the pearlitic spacing (arising from the confined slip of dislocations in the lamellae) and on strengthening from the evolving intra-lamella dislocation density. A Kocks-Mecking strain hardening/recovery model is used for the lamellar ferrite, whereas perfect-plastic behaviour is assumed for cementite. The model naturally captures the microstructural evolution and the internal micro-stresses developed due to the different mechanical behaviour of both phases. The model is also able to describe the lamellar evolution (orientation and interlamellar spacing) with good accuracy. The role of plastic anisotropy in the ferritic phase has also been studied, and the results show that anisotropy has an important impact on both microstructural evolution and strengthening of heavily drawn wires.

1. Introduction

The eutectoid Fe-C pearlite is an aggregate of composite colonies constituted of bcc ferrite lamellae alternating with lamellae of orthohombic cementite (Fe₃C iron carbide). Cementite occupies approx. 12% of the volume. The lamellae are approximately flat and continuous, although the real geometry always contains growth defects (lamellar discontinuities, and deviations from planarity). The as-transformed pearlitic spacing (λ) depends on the transformation temperature (on the undercooling with respect to the equilibrium eutectoid temperature), and in general falls in the range 50 nm < λ < 600 nm. The colony size is often 10 or 20 times the pearlitic spacing or even more.

Each as-transformed colony is an intertwined two-phase bicrystal. It is well known that the strength of pearlitic steels is related to the interlamellar spacing through a Hall-Petch type empirical relationship. This is explained by the critical bowing of dislocation lines necessary to achieve long-range slip on its slip plane confined between two adjacent cementite lamellae [1-6].

The anisotropic behaviour of pearlite stems from both crystallographic and geometric origins. The two-phase continuum model proposed in this work deals strictly with the latter, assuming that plastic anisotropy of the ferrite arises only from its lamellar structure. The model is intended for practical use in plastic forming simulations of pearlitic steel. Its good predictive capabilities, even when strain-path
changes are assumed, indicate that in pearlite anisotropy from a geometrical origin dominates over that related to crystallographic texture.

2. Model
The model combines a Hill-based material description accounting for the plastic anisotropy of ferrite due to the confined slip of dislocations in the lamellae and an isotropic elastic- perfectly plastic von Mises plasticity model for cementite. The model assumes perfect adhesion between cementite and ferrite lamellae. The model also assumes identical isotropic elastic properties for both phases.

2.1. Model for ferritic lamellae
In pearlitic ferrite, the plastic deformation is controlled by dislocation glide confined between the two neighbouring cementite lamellae. The stress $\tau_{\alpha\alpha}$ allowing long-range slip is assumed to be composed of additive contributions from any kind of friction-like resistance (i.e. the true lattice friction stress and a contribution from solution strengthening), $\tau_0$, as well as from the bowing of dislocation lines between the cementite walls or ferritic grain boundaries, $\Delta \tau_{\text{bow}}(s_{\text{eff}})$, where $s_{\text{eff}}$ is the effective interlamellar spacing which, in principle, depends on the orientation of the applied stress, and from the resistance offered by the presence of a strain-dependent dislocation density, $\Delta \tau_{\rho}$, i.e.,

$$\tau_{\alpha\alpha} = \tau_0 + \Delta \tau_{\text{bow}}(s_{\text{eff}}) + \Delta \tau_{\rho}$$

(1)

The model accounts for this yield anisotropy with a simple Hill model. The anisotropic yield locus proposed by Hill in 1948 [7] is the simplest extension of the von Mises yield criterion, i.e., a quadratic expression that can be written as

$$f = \sigma_{\text{eff}}^2 - \sigma_0^2 = \frac{1}{2} \sigma^T P_H \sigma - \sigma_0^2$$

(2)

where,

$$P_H = \begin{pmatrix}
  \alpha_{12} + \alpha_{31} & -\alpha_{12} & -\alpha_{31} & 0 & 0 & 0 \\
  -\alpha_{12} & \alpha_{12} + \alpha_{23} & -\alpha_{23} & 0 & 0 & 0 \\
  -\alpha_{31} & -\alpha_{23} & \alpha_{23} + \alpha_{31} & 0 & 0 & 0 \\
  0 & 0 & 0 & 6\alpha_{44} & 0 & 0 \\
  0 & 0 & 0 & 6\alpha_{55} & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 6\alpha_{66}
\end{pmatrix}$$

(3)

and

$$\begin{align*}
\alpha_{12} &= \left(\frac{\sigma_0}{\sigma_{11}}\right)^2 + \left(\frac{\sigma_0}{\sigma_{22}}\right)^2 - \left(\frac{\sigma_0}{\sigma_{33}}\right)^2 ; \\
\alpha_{23} &= \left(\frac{\sigma_0}{\sigma_{11}}\right)^2 + \left(\frac{\sigma_0}{\sigma_{33}}\right)^2 - \left(\frac{\sigma_0}{\sigma_{22}}\right)^2 ; \\
\alpha_{31} &= \left(\frac{\sigma_0}{\sigma_{11}}\right)^2 + \left(\frac{\sigma_0}{\sigma_{22}}\right)^2 - \left(\frac{\sigma_0}{\sigma_{33}}\right)^2 ;
\end{align*}$$

(4)

$$\begin{align*}
3\alpha_{44} &= \left(\frac{\sigma_0}{\sigma_{12}}\right)^2 \\
3\alpha_{55} &= \left(\frac{\sigma_0}{\sigma_{23}}\right)^2 \\
3\alpha_{66} &= \left(\frac{\sigma_0}{\sigma_{31}}\right)^2.
\end{align*}$$

where $\sigma_{ij}$ are the uniaxial/shear yield stresses. Particularized for the so-called “normal anisotropy” (transversely isotropic materials), i.e., planar isotropy in lamellar plane, e.g., the (1, 2) plane, $\sigma_{11} = \sigma_{22} = \sqrt{3} \sigma_{12}$ and $\sigma_{31} = \sigma_{23}$. Thus, equation (2) reduces to
\[ f = \sigma_2^2 - \sigma_1^2 = \frac{1}{2} \sigma^TP_H \sigma - \sigma_1^2 = 0 \]  

(5)

with

\[
P_H = \begin{pmatrix}
2 & N - 2 & -N & 0 & 0 & 0 \\
N - 2 & 2 & -N & 0 & 0 & 0 \\
-N & -N & 2N & 0 & 0 & 0 \\
0 & 0 & 0 & 6M & 0 & 0 \\
0 & 0 & 0 & 0 & 6M & 0 \\
\end{pmatrix}
\]

(6)

where \( M = \sigma_{12}^2 / \sigma_{23}^2 \) and \( N = \sigma_{11}^2 / \sigma_{33}^2 \). It is easy to see that as the active gliding dislocations under \( \sigma_{12} \) shear stresses are confined between two cementite lamellae, then a minimum \( s_{\text{eff}} = s \) (\( s \) being the interlamellar spacing) should be considered in equation (1). Thus, we can anticipate that \( M = \sigma_{12}^2 / \sigma_{23}^2 \geq 1 \); a similar argument leads to \( N = \sigma_{11}^2 / \sigma_{33}^2 \geq 1 \). Implicitly, and compared with a crystal plasticity approach, the model assumes that slip may occur along any crystal direction and plane, and that the critical shear stress is minimum along lamellar planes (\( \sigma_{31} = \sigma_{23} \leq \sigma_{12} \)). Particularly, when \( M = N = 1 \), pearlitic ferrite is fully isotropic (von Mises behaviour).

2.2. Model for cementite lamella

Cementite is considered to be mechanically isotropic with elastic-perfectly plastic behaviour (\( Y = 4500 \) MPa).

2.3. Interphase boundaries

Perfect adhesion is considered between cementite and ferrite. Thus, equivalent in-plane displacements and equivalent out-of-plane stresses are assumed on both sides of the boundary.

2.4. Microstructural evolution

The model assumes that plastic flow directly determines the orientation and spacing of the lamellae. Thus, the normal orientation of each lamella is given by

\[
\hat{n} = \frac{F^{-T}\hat{n}_0}{\sqrt{F^{-T}\hat{n}_0}}
\]

(7)

where \( \hat{n}_0 \) is the initial orientation of the lamella normal and \( F \) is the deformation gradient. Likewise, the interlamellar spacing is calculated as follows:

\[
s = \frac{s_0}{\sqrt{F^{-T}\hat{n}}}
\]

(8)

where \( s_0 \) is the initial lamellar spacing. The model was implemented in a VUMAT subroutine for ABAQUS®/Explicit.

3. Uniform elongation with periodic boundary conditions

In order to check the capabilities of the proposed model and to verify the relevance of the anisotropic model for pearlitic ferrite, the same uniform elongation with periodic boundary conditions was simulated for a fully isotropic ferritic model \( (M = N = 1) \) and for an anisotropic ferritic model \( (M, N > 1) \) considering that gliding dislocations for \( \sigma_{31} \)-type shear stresses are only confined by the colony size,
i.e., $s_{eff} = c = 10 \, \mu m$ in equation (1). Assuming a homogeneous initial inter-lamellar spacing of $s = 60$ nm, an initially cubic mesh with 25x25x25 elements was constructed with a Voronoi tessellation to mimic an equiaxed cluster of approximately 100 randomly oriented pearlite colonies (see figure 1).

**Figure 1.** Coloured representation of the initial colony distribution in the designed mesh.

The virtual microstructure was uniaxially elongated with periodic boundary conditions up to an equivalent strain of about 4. Figure 2 shows a top view perpendicular to the loading direction (direction 3) after uniaxial elongation for the isotropic ferritic model (centre) and the anisotropic ferritic model (right). The results show that the deformation is quite homogeneous in the isotropic model and that colonies maintain a near self-similar shape even after severe elongation. In contrast, the anisotropic model leads to a heavily distorted mesh with colonies stretched in a way that reproduces the typical “van Gogh skies structure” observed in heavily drawn bcc wires [8, 9].

**Figure 2.** Top view perpendicular to the loading direction of the obtained mesh after a true strain about 4 (macroscopically axisymmetric elongation). Left: Initial mesh re-scaled; Centre: Mesh after maximum elongation for the isotropic ferritic model; Right: Idem for anisotropic ferritic model. Colour code represents the Y direction cosine of the normal to the lamellae.
Figure 3. Evolution of normalized interlamellar spacing with applied equivalent strain for the simulated uniform elongation. Blue line: anisotropic ferritic model; red line: isotropic ferritic model; green line: evolution of mean interlamellar spacing of a randomly oriented distribution of pearlitic colonies assuming a homogeneous distribution of strain with equations (7) and (8). Symbols: experimental measurements of normalized interlamellar spacing for pearlitic wires drawn to different equivalent strains [1, 3, 10, 11].

With regard to the colony refinement, figure 3 shows the evolution of the normalized mean interlamellar spacing with equivalent strain for both models (red for the isotropic model, and blue for the anisotropic model). The results are compared with normalized experimental interlamellar spacings (symbols) at equivalent levels of drawing strain. The results show that the proposed anisotropic model (blue line) reproduces the evolution of spacing very accurately and better than the isotropic model. Moreover, the evolution for the isotropic model is very similar to that expected from homogeneous deformation (i.e., the evolution of mean interlamellar spacing considering a homogeneous deformation gradient and equations (7) and (8); see green line in figure 3).

The results in figures 2 and 3 implicitly show that the re-orientation of the colonies, and the evolution of the microstructure, is not as trivial as that described by the isotropic ferritic model. The proposed anisotropic model, in contrast, captures well the microstructural evolution.

Figure 4 shows a stereographic projection of lamellar normals at different equivalent applied strains. Again, the model reproduces the evolution of lamellar orientations as expected under uniaxial loading, namely that all the normals should re-orient perpendicular to the loading direction. The qualitative evolution of the orientation of the lamellae is quite similar for both models, but the anisotropic model promotes internal orientation spreading within colonies, and a random dispersion of orientations around the equator, which can be understood as an effect of colony curling.

With regard to the mechanical response, figure 5 shows the stress-strain curve and the work hardening slope (i.e., the derivative of the true stress with respect to the equivalent strain) for both models. The curves show three different regions. The very first part of the curves (see magnified region in figure 5) shows an elastic loading followed by a linear hardening until real yielding occurs. This “double yielding” is due to the different yield limits of ferrite and cementite. In a real experiment, this double yielding is difficult to see due to the heterogeneity of interlamellar spacings in pearlite that leads to different local critical shear stresses. The second part of the curve (0.1 < \( \varepsilon_{eq} \) < 2) shows a decreasing work hardening until it stabilizes around 400-500 MPa for the anisotropic model. At this stage, the ferrite work hardens following a Voce-type hardening, and the colonies re-orient as shown in figure 4. Finally,
for $\varepsilon_{\text{eq}} > 2$, the colonies stretch as shown in figure 2 while the interlamellar spacing drops below 20 nm. The curve at this stage shows an increasing work hardening behaviour (>1 GPa for the anisotropic model).

Figure 4. Stereographic projection of the lamellar normals for, $\varepsilon_{\text{eq}}$ = 0.1, 1 and 4 (left to right). Upper row: Isotropic ferritic model; Bottom row: Anisotropic ferritic model. Blue and red points correspond to normals belonging to the upper and lower hemispheres, respectively.

Figure 5. Left: True stress vs true strain curve for the simulated uniform elongation with periodic boundary conditions up to an equivalent strain of $\sim 4$. The box shows a magnified detail of the elastic region showing a “double yielding” behaviour. Right: Work hardening rate as a function of the applied equivalent strain.

Even though these three stages are seen in both the isotropic and anisotropic models, there are some clear differences in the stress-strain curves. Firstly, the curves intersect at $\varepsilon_{\text{eq}} \sim 1.3$. At low strains the isotropic model shows higher flow stresses than the anisotropic model as expected (note that for the anisotropic model, $N, M > 1$, i.e., the flow stress is lower for the out-of-plane components). In contrast, as deformation progresses, the anisotropic model shows a much higher work hardening rate than the isotropic model. This is due to the curling of the pearlitic colonies (figure 2), which reduces the mean
interlamellar spacing (figure 3) and, thus, increases the strength of the pearlitic steel according to equation (1).

Figure 6. Difference between the ultimate tensile strengths of drawn wires over patented wires ($\Delta TS$) vs the corresponding drawing strain. Open black symbols correspond to a compilation of experimental tests published by Lesuer et al. [12] and blue symbols correspond to experimental data obtained by Zhang et al. [13] on steel wires supplied by Bekaert. Superposed in blue (anisotropic) and red (isotropic), are the simulated stress curves of figure 5, from which the initial part of the curve has been subtracted.

The anisotropic model is in good correspondence with the experimentally observed evolution of strength of heavily drawn wires. Figure 6 shows the difference between the ultimate tensile strengths of drawn wires over patented wires (\( \Delta TS \)) vs the corresponding drawing strain. Superposed in blue and red are the simulated stress curves from which the first part of the curve has been subtracted. The anisotropic model reproduces perfectly the strengthening of drawn wires even beyond the expected limits of the model (above equivalent strains of 2.5) where dissolution of cementite is expected.

4. Conclusions
- A new relatively simple mesoscopic numerical model has been proposed that describes accurately both the mechanical behaviour and the microstructural evolution of lamellar multi-colony pearlite. The model has been validated with experimental results obtained from literature in heavily drawn wires.
- The model confirms the key role of the anisotropic properties of the ferritic phase on the development of the microstructure, and on the strengthening ability, of heavily drawn wires.

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References
[1] Embury A D and Fisher R M 1966 Acta Metall. 14 147-159
[2] Langford G 1970 Metall. Trans. 1 465-477
[3] Langford G 1977 Metall. Trans A 8A 862-875
[4] Gil Sevillano J 1979 ICSMA 5 Proc. vol 2, ed P Haasen, V Gerold et al. (Oxford UK: Pergamon Press) p 719
[5] Gil Sevillano J 2011 Wire Journal International 44 58-70
[6] Borchers C and Kirchheim R 2016 Progr. Mater. Sci 82 405-444
[7] Hill R 1948 Proc. Roy. Soc. London, 193 281–297
[8] Gil Sevillano J, Matey Muñoz L and Flaquer Fuster J 1998 J. Physique IV 8 155
[9] Gil Sevillano J, García-Rosales C and Flaquer Fuster J 1999 Phil. Trans. R. Soc. London A 357 1603-1619
[10] Matschass F 1988 Wiss. Z. Techn. Univ. Magdeburg 32 21-28
[11] Zhang X, Hansen N, Godfrey A and Huang X 2016 Acta Mater. 114 176-183
[12] Lesuer D R, Syn C K, Sherby O D and Kim D K 1966 Lawrence Livermore Nat. Lab. UCRL-JC-124374
[13] Zhang X, Godfrey A, Huang X, Hansen N and Liu Q 2011 Acta Mater. 59 3422-3430