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Generalization of the existing relations between microstructure and yield stress from ferrite–pearlite to high strength steels

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A series of available equations allows the yield and the tensile strength of low carbon ferrite–pearlite microstructures to be expressed as a function of the optical grain size, steel composition and interstitials in solution. Over the years, as the complexity of steel microstructures has increased, some additional terms have been added to account for precipitation and forest dislocation contributions. In theory, this opens the door for an extension of these equations to bainitic microstructures. Nevertheless, there is a series of difficulties that needs to be overcome in order to improve prediction accuracy. In the present work, different microstructures (ferrite–pearlite, bainite, quenched, and quenched and tempered) were produced and tension tested in a C–Mn–Nb steel. Optical microscopy and EBSD (Electron Back Scattered Diffraction) were applied and the results were compared as a function of the tolerance angle. Based on this work, an adaptation to Pickering's equation is proposed, including its extension to other microstructures rather than ferrite–pearlite.

1. Introduction

The easiest and most widely used approach to predicting basic tensile properties of low carbon ferrite–pearlite microstructures involves a number of empirical equations like those that express yield stress, σ_y, as a function of different strengthening contributions [1–6]:

$$\sigma_y = \sigma_0 + \sigma_{ss} + \sigma_{iss} + \sigma_{pre} + \sigma_\rho + \sigma_d \tag{1}$$

In this equation, σ_0 is the Peierls–Nabarro stress or lattice friction stress, σ_{ss} and σ_{iss} are the short range internal stresses produced, respectively, by substitutional and interstitial elements in solid solution, σ_{pre} is the contribution of the precipitates, σ_ρ is the contribution of forest dislocations and $\sigma_{d,}$ is the contribution of the ferrite grain size, *d*.

It is usually considered thought that the contribution of an element in solution is independent of the presence of other elements and that it produces an increase in strength proportional to its concentration [1,7–11]. Substitutional elements produce a moderate strengthening as compared to interstitial atoms like carbon and nitrogen, whose contribution, $\sigma_{iss,}$ is enhanced by their strong interaction with dislocations [12,13].

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The contribution of the grain boundaries to the strength follows a Hall–Petch relationship [1–5]:

$$\sigma_d = k_{HP} d^{-1/2} \tag{2}$$

For ferrite, k_{HP} adopts values between 15 and 18 (MPa mm$^{0.5}$) when d is expressed as the mean linear intercept (MLI) measured by optical microscopy [5]. Pickering's equation, which applies to air-cooled mild steels, incorporates a value of k_{HP}=17.4 MPa mm$^{0.5}$ [1,7], leading to [1,7,14]:

$$\sigma_y = 54 + 32\text{Mn} + 678\text{P} + 83\text{Si} + 39\text{Cu} - 31\text{Cr} + 11\text{Mo} + 5000(\text{C}_{free} + \text{N}_{free}) + 17.4d^{-0.5} \tag{3}$$

in which the concentrations of the different elements are expressed in wt%. As an alternative, Choquet et al. proposed an equation in which k_{HP} varies with the C and Mn content and with the fraction of ferrite [15].

Some authors have proposed non-linear relations hold for microalloyed steels, instead of a linear equation like Eq. (1). For example, the joint effect of dislocations and precipitation has been considered by using a Pythagorean flow stress addition law term, while Hall–Petch and solute contributions were treated as usual [16]. This non linear term accounting for the strengthening contribution of forest dislocations and precipitates is theoretically supported by the computer simulations made by Foreman and Making [17] and requires a similar density of relatively weak and strong obstacles on the slip plane. The non linear equation proposed by Bouaziz et al. [18] is another empirical variant that includes into the Pythagorean addition law term all the strengthening contributions (solutes, Niobium hardening and ferrite work hardening), excepting the Hall–Petch term. This to show that there is no unanimity in the form of the proposed non-linear laws, nor available information showing that they have been tested on a large set of conditions. In contrast, the linear approach has a higher experimental support and apparently, after having been tested on a large set of microalloyed steels, it seems reasonably accurate as reported in Ref. [19].

The Hall–Petch equation was initially derived for high angle boundaries, but it was progressively extended to subgrains [20] and cell boundaries [21]. Nevertheless, the strengthening due to the sub-boundaries depends on their misorientation, and it can eventually lead to a modified Hall–Petch exponent. In general, the strength of the sub-boundaries is lower than that of the grain boundaries, but a critical misorientation angle at which the strength of the dislocation boundary equals that of a high angle boundary can be defined. Some calculated critical angle values are quite small ($\sim$0.2 to 2°) and a value of about 0.52° was estimated for an interstitial free (IF) steel [22]. However, there is no theoretical support for these low angles that could be the result of the relatively low Hall–Petch slopes in the considered materials [22].

For cell size hardening, the Langford–Cohen (L–C) model ($\sigma_d = k_{LC}\, d^{-1}$) is usually applied instead of the Hall–Petch equation [23]. Bainite and martensite laths have low angle boundaries and both L–C and H–P models have been applied, depending on the author. For example, Norström proposed for tempered martensite the following equation [24]:

$$\sigma_y = \sigma_0 + \sigma_{iss} + k_y D^{-0.5} + k_s d^{-0.5} + \alpha M \mu b [\rho_0 + K(\%C)]^{0,5} \quad (4)$$

in which, k_y, k_s and K are constants, D is the packet size, d is the lath width, $\alpha M = 0.7$, μ is the shear modulus, b is the Burgers vector, ρ_0 is the dislocation density of martensitic pure iron and (%C) is the carbon content. This equation assumes H–P model applies to both high angle boundaries (packet) and lath boundaries. The lath size in this work is of $\sim$0.3 μm. Naylor suggested that, as long as the effective lath size was not larger than 1 μm, a relation $\sigma_d \propto M^{-1}$ applies instead of the H–P relation [25]. Based on transmission electron microscopy measurements, this same author deduced the following expression for low carbon bainite and tempered martensite [25]:

$$\sigma_d = 450 d_M{}^{-1} \quad (5)$$

in which d_M is equivalent to the MLI. A variant of this equation has recently been proposed, incorporating the effective lath size width instead of using d_M [26].

The relatively recent incorporation of the EBSD techniques allows the mesotexture of steels to be determined and grain boundaries to be discriminated in terms of their misorientation. This new microstructural characterisation capacity can be used to improve the relationships between the microstructure and the mechanical properties. It has been found, for example, that a thermomechanically processed steel presents a high concentration of low angle boundaries as a result of a variant selection that takes place during transformation [27,28].

One of the main fields of application for EBSD techniques is the area of the complex high strength steel microstructures produced in modern steels, which cannot be properly quantified by means of the optical microscope due to their fineness [29]. In this field, EBSD is being increasingly applied, but some questions need to be solved via systematic investigation. The first issue is that even for simple ferrite microstructures, optically measured grain sizes can be significantly different from those obtained by EBSD [30]. The uncertainty about how to compare optical and EBSD results is translated into the most conventional microstructure-mechanical property equations that are traditionally tuned on optically measured grain sizes. When increasing the complexity of the microstructure, new problems appear, most of which are related to the resolution of the EBSD technique used to detect low angle boundaries defining the ferrite sub-units within the packets and sheaves and to how to quantify the microstructure (i.e., define a minimum threshold angle). When these difficulties are overcome, a question still remains as to how to apply the available equations relating microstructural parameters to the yield, tensile strength and transition temperature when using EBSD results. The present work concentrates on yield strength and addresses most of these points with the aim of extending the applicability of the available equations to complex steel microstructures.

2. Experimental

A broad range of microstructures has been produced by different thermal and thermomechanical sequences on a Nb-microalloyed steel, with the composition shown in Table 1. Details about the laboratory thermomechanical simulations are described as follows:

- *Plane strain compression tests + controlled cooling and simulated coiling:* the steel was reheated at 1200 °C and held at this temperature for 30 min, followed by cooling to the deformation temperature, where one or two deformation passes were applied in order to condition the austenite. The details for these sequences are as follows:
  - Sequence 1 (S1): deformation at 1100 °C and 1 s^{-1} to a strain of 0.5, followed by 5 s holding in order to recrystallise the austenite and a final cooling to the coiling temperature.
  - Sequence 2 (S2): deformation at 1100 °C and 1 s^{-1} to a strain of 0.5, plus 5 s holding at 1100 °C, followed by a deformation pass at 950 °C and 1 s^{-1} to a strain of 0.3, followed by cooling to the coiling temperature.
  - Water quenching after both thermomechanical sequences instead of coiling, producing samples identified as S1-Q and S2-Q, respectively.
- *Horizontal-vertical compression tests + controlled cooling and simulated coiling:* Horizontal–vertical compression tests were performed in order to accumulate strain in austenite during thermomechanical processing. After reheating at 1200 °C for 30 min, four deformation passes were applied with a total absolute strain of 1.7 according to the following sequence:
  - Sequence 3 (S3): Deformation at 1 s^{-1} in four passes: at 1100 °C to ε=0.4, at 1050 °C to ε=0.4, at 975 °C to ε=0.4 and at 900 °C to ε=0.5, followed by cooling to the coiling temperature.

Independently of the thermomechanical sequence, coiling was simulated by 1 h of holding at the coiling temperature

Table 1
Chemical composition (wt, %).

C	Si	Mn	P	S	Al	Nb	V	N	Mo	Cu	Cr	Ni
0.15	0.30	1.42	0.012	0.002	0.037	0.033	0.011	0.007	0.003	0.012	0.02	0.03