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# A physical model of the twinning-induced plasticity effect in a high manganese austenitic steel

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## Abstract

The steel Fe–22 wt.% Mn–0.6 wt.% C exhibits a low stacking fault energy (SFE) at room temperature. This rather low value promotes mechanical twinning along with strain which is in competition with dislocation gliding, the so called twinning-induced plasticity effect. The proposed modeling of the mechanical behavior introduces the formation of mechanical microtwins in a viscoplasticity framework based on dislocation glide at the mesoscopic scale in the case of a simple tensile test. The important parameter is the mean free path of the dislocations between twins, whose reduction explains the high hardening rate (by a dynamical Hall–Petch-like effect). It takes into account the typical organization of microtwins observed in electron microscopy (geometrical organization by using a twin-slip intersection matrix). To take into account the polycrystalline disorder, the macroscopic flow stress is calculated by assuming that the deformation work is equal in each grain for each strain step. This model gives an intermediate rule between Taylor and Sachs approximations and is simpler to compute than self-consistent methods. The parameters for gliding are first fitted on results at intermediate temperatures (without twinning), and the whole modeling is then correlated at room temperature. The simulated results (microstructure and mechanical properties) are in good agreement with experience.

*Keywords:* TWIP effect; Mecking–Lücke; IsoW; Twinning; Viscoplasticity

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## 1. Introduction

The main industrial interest of low stacking fault energy (SFE) fcc steels is their capability to provide a high work hardening rate, a good ductility and a high-strength during mechanical loading. These engineering high-strength steels are mostly devoted to automotive bodies, where the challenge consists in designing lightweight automobiles [1].

These exceptional characteristics are achieved by mechanisms involving interactions between slip, mechanical twinning and also in some conditions martensitic transformation [2]. Consequently, the deformation microstructure of these materials can be quite complex. These austenitic steels have been the focus of intense experimental and theoretical studies [3–6]. In this paper, we exploit an approach

alternative to a self-consistent framework which was first proposed by Bouaziz and Buessler [7] in which is introduced the formalism proposed by Bouaziz and Guelton [8].

The austenitic Fe–22 wt.% Mn–0.6 C wt.% steel used in this study exhibits a low SFE at room temperature [2]. This rather low value promotes mechanical twinning in competition with gliding along with strain. Since the volume fraction of twins increases with strain, the mean free path of dislocations decreases rapidly. The resulting high hardening rate delays necking during tensile tests. This hardening effect due to mechanical twinning is known as twinning-induced plasticity (TWIP) [1]. Thus, the studied grade shows simultaneously high elongation to fracture (70%) and tensile strength (1200 MPa) [2,9].

In this paper, we use the results of an experimental study presented elsewhere [9] and particularly the observed multiscale organization of twinning and orders of magnitude. In the following, the equations are written using Einstein's convention.

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## 2. Modeling at the mesoscopic scale

We first model the behavior of a grain oriented with respect to the tensile direction (tensile stress  $\sigma$ ).

### 2.1. Constitutive laws and hypotheses for slip

Twenty-four slip systems are introduced in each grain. These systems correspond to the 24 potential perfect dislocation systems.  $b_{110}$  is the Burgers vector for these perfect dislocations. These slip systems are characterized by their Schmid factor  $ms_i$  ( $i = 1, 24$ ) and the stored dislocation density  $\rho_i$  ( $i = 1, 24$ ) which are the internal state variables of the grain.

Dislocation of a given system  $i$  can move through the forest when the resolved shear stress  $\tau_i$  overcomes  $\tau_i^{c\text{-slip}}$ , calculated using the Franciosi interaction matrix and the dislocation densities stored in the other systems:

$$\tau_i^{c\text{-slip}} = \tau_0 + \alpha\mu b_{110}\sqrt{A_{ij}\rho_j} \quad (1)$$

with  $\alpha$  a parameter which characterizes the resistance of the forest ( $\alpha = 0.4$ ),  $\mu$  the shear modulus,  $\tau_0$  a friction stress due to carbon and  $[A]$  a symmetric ( $24 \times 24$ ) slip–slip interaction matrix first proposed by Franciosi [10] and defined as follows:  $A_{ij} = 0.7$  if  $i$  and  $j$  represent the same system or its inverse. This term is not set equal to 0 to partially model the backstress due to the stress relaxation of the system itself,  $A_{ij} = 0.4$  if  $i$  and  $j$  are collinear, coplanar, or perpendicular,  $A_{ij} = 0.75$  if the systems  $i$  and  $j$  form mobile junction,  $A_{ij} = 1$  if the systems  $i$  and  $j$  form Lomer–Cottrell locks. For a given system  $i$ , the effective resolved shear stress  $\tau_i^{\text{eff}}$  is the effective stress acting on the dislocations, i.e.  $\tau_i^{\text{eff}} = \tau_i - \tau_i^{c\text{-slip}}$ . Following the viscoplastic approach proposed by Conrad and Narayan [11], the shear rate  $\dot{\gamma}_i$  produced by system  $i$  under this effective stress is given by:

If  $\tau_i^{\text{eff}} > 0$

$$\text{then } \dot{\gamma}_i^{\text{slip}} = \dot{\gamma}_0 \exp\left(-\frac{\Delta G}{k_B T}\right) \sinh\left(\frac{\tau_i^{\text{eff}} V_i^{\text{a-slip}}}{k_B T}\right) \quad (2)$$

with  $\dot{\gamma}_0$  a reference shear rate,  $\Delta G$  the activation energy for slip,  $k_B$  Boltzmann's constant,  $T$  the temperature and  $V_i^{\text{a-slip}}$  the activation volume. Since the density of forest dislocations for a given system  $i$  increases along with strain, we empirically model the decrease of the activation volume by

$$V_i^{\text{a-slip}} = b_{110}^3 \frac{\tau_{VA}}{\tau_i^{c\text{-slip}}} \quad (3)$$

with  $\tau_{VA}$  a normalizing parameter.

According to the literature [12–14], the density of dislocations evolves with the reduction of the mean free path (MFP)  $\Lambda_i$ .

$$\frac{d\rho_i}{d\gamma_i} = \frac{1}{b_{110}\Lambda_i} - f\rho_i \quad (4)$$

with  $f$  a parameter which accounts for dynamical recovery. Without twinning, the MFP is calculated with a harmonic mixing law accounting for the obstacles seen by the dislocations, i.e. the grain boundaries and the dislocations of the forest:

$$\frac{1}{\Lambda_i} = \frac{1}{D} + k\sqrt{A_{ij}\rho_j} \quad (5)$$

with  $D$  the effective grain size and  $k$  a constant which reflects the relative hardening between grain boundaries and dislocations of the forest.

### 2.2. Microstructure refinement by twinning

To describe twinning, we introduce the 12 twinning systems, which can be activated in a fcc alloy. They are described by their pseudo Schmid factor  $mt_i$  corresponding to the 12 possible Shockley dislocations [9] and by their partial volume fraction  $f_i$ . The partial fractions of twins are also to be considered as internal state variables.

Microtwins are stored into stacks (see [9]) and are strong obstacles for dislocation gliding as grain boundaries. For a given gliding system  $i$ , the MFP becomes:

$$\frac{1}{\Lambda_i} = \frac{1}{D} + \frac{1}{t_i} + k\sqrt{A_{ij}\rho_j} \quad (6)$$

with  $t_i$  the MFP between microtwins secant to the slip system (coplanar twins are not taken into account).

To evaluate this refinement, we set up the distance  $d_j$  which is the distance between two microtwin stacks of a given twinning system  $j$ . The MFP  $t_i$  for the slip system  $i$  is evaluated using an harmonic mixing law:

$$\frac{1}{t_i} = B_{ij} \frac{1}{d_j} \quad (i = 1, 24 \text{ and } j = 1, 12) \quad (7)$$

with  $[B]$  a symmetric ( $24 \times 12$ ) slip–twin intersection matrix defined using the following rules:  $B_{ij} = 0$  if  $i$  and the twinning system  $j$  are coplanar,  $B_{ij} = 1$  if  $i$  and the twinning system  $j$  are secant.

In the same manner we define the MFP  $l_j$  for a given twinning system  $j$ . This distance corresponds to the length along which newly created twins on this system could extend. Since grain boundaries and twins of the secant twinning systems are strong obstacles for a given twinning system, the parameter is described using the same formalism.

$$\frac{1}{l_j} = \frac{1}{D} + B'_{ij} \frac{1}{d_j} \quad (8)$$

with  $[B']$  a ( $12 \times 12$ ) twin–twin intersection matrix defined using the same rules as for  $[B]$ .

The volume of the newly created twins assuming a penny shape is given by:

$$V_i = \frac{\pi}{4} D l_i e_i \quad (9)$$

with  $e_i$  the mean thickness of the microtwins.

The distance between coplanar microtwin stacks of a given system [4] is computed using a modified Fullman's stereological relationship [9].

$$\frac{1}{d_i} = \frac{f_i}{n_i e_i (1 - F)} \quad (10)$$

with  $F$  the total fraction of twins and  $n_i$  the mean number of microtwins in a stack.

Finally, Eq. (6) can be specified accounting for the different kinds of obstacles for the dislocations, i.e. grain boundaries, secant twin boundaries and forest dislocations respectively:

$$\frac{1}{\Lambda_i} = \frac{1}{D} + \frac{1}{1 - F} B_{ij} \left( \frac{f_j}{e_j n_j} \right) + k \sqrt{A_{ik} \rho_k} \quad (11)$$

### 2.3. Constitutive law for twinning

As twinning is a displacive transformation, the evolution of the volume ratio of twins for a given system  $i$  is given by [4,15]:

$$\frac{df_i}{1 - F} = V_i dN_i \quad (12)$$

with  $dN_i$  the number of newly created twins during the strain increment.  $V_i$  is geometrically determined using Eq. (9).

#### 2.3.1. Modeling of the critical shear stress for twinning

As described in the literature, twinning occurs only when the applied resolved shear stress reaches a certain critical value (CRSS). Many authors develop their own modeling of the CRSS [3,16,17]. A force balance on the twinning dislocation is commonly used at the scale of twin nucleus.

The different forces acting on the twinning dislocations are due to [3,16,18,19]: (i) the back-stress due to the extension of a stacking fault, (ii) the self-stress due to dislocations curvature, (iii) the internal stress concentration due to other dislocations pile-ups.

According to our formalism, these three contributions are integrated using an additive formalism as [3]:

$$\tau_i^{\text{c-twin}} = \tau^{\text{c-int}} + \tau_i^{\text{curvature}} - \tau_i^{\text{pile-ups}} \quad (13)$$

The intrinsic term  $\tau^{\text{c-int}}$  is proportional to the SFE. The higher the SFE, the higher the CRSS [17,18]. The last contribution is due to dislocation pile-ups which act as stress concentrators for twin nucleation.

#### 2.3.2. Twinning kinetic

Twins nucleation requires high stress concentrations which are provided by dislocation pile-ups on strong obstacles. We locate the twin embryo only on such obstacles. For a given twinning system  $i$ , the specific surface for nucleation is evaluated as follows:

$$\frac{S_i^{\text{interface}}}{D^3} = \frac{1}{l_i} \quad (14)$$

At the very beginning of loading,  $S^{\text{interface}} = D^2$  and when a secant twinning system appears, more interfaces are available for nucleation which is consistent with Eq. (8).

Following a viscoplastic approach and introducing Eq. (14), we presume a kinetic law:

$$\text{If } mt_i \sigma > \tau_i^{\text{c-twinning}} \text{ then } \dot{N}_i = \frac{G}{l_i} (mt_i \sigma - \tau_i^{\text{c-twinning}}) \dot{\epsilon} \quad (15)$$

with  $\dot{\epsilon}$  the strain rate of the grain since twin nucleation requires prior plastic deformation and  $G$  a constant.

Finally, the total shear strain in the given grain under the tensile stress  $\sigma$  is the sum of the two contributions: slip in the untwinned austenite and twinning:

$$\dot{\epsilon} = (1 - F) m s_i \dot{\gamma}_i^{\text{slip}} + \frac{1}{\sqrt{2}} m t_i \dot{f}_i \quad (16)$$

Even if numerous twins nucleate, the total fraction of twins is very low since the microtwins are of a few tenth of nanometer thick. Thus, the plastic deformation is mainly achieved by dislocation gliding.

## 3. Homogenization law

The polycrystal is assumed to be an aggregate of grains randomly oriented with respect to the tensile direction. The macroscopic flow stress is calculated by assuming that the mechanical work increment is equal in each grain for each strain step (IsoW assumption developed by Bouaziz and Buessler [7]). This model gives an intermediate rule between the Taylor and Sachs approximations

$$\forall \varphi, \theta \quad \sigma_\varphi(\varepsilon_\varphi) d\varepsilon_\varphi = \sigma_\theta(\varepsilon_\theta) d\varepsilon_\theta \quad (17)$$

where  $\varphi$  and  $\theta$  are orientation indices. The macroscopic strain and flow stress are averaged over the whole grains.

## 4. Results of the model for the studied steel

Several tensile tests were carried out at room temperature after pre-strain at 673 K. Since the SFE increases with temperature, mechanical twinning does not occur at this temperature. The plot of the elastic limits vs. the prestrain at 673 K is use as the stress-strain curve the alloy would have at room temperature in the absence of TWIP effect. The parameters (see Eqs. (1), (2) and (5)) for gliding are first fitted on such results and on results at 673 K. The whole modeling including twins is then correlated with the experimental results at room temperature.

Fig. 1 presents the stress-strain tensile curve of the alloy (grain size of 20  $\mu\text{m}$ ) at room temperature and at 673 K. The model is applied in both cases with the same set of parameters except for the temperature and the SFE [2] which is set high enough at 673 K to inhibit twinning. The most relevant parameters used for the simulation are summed up in

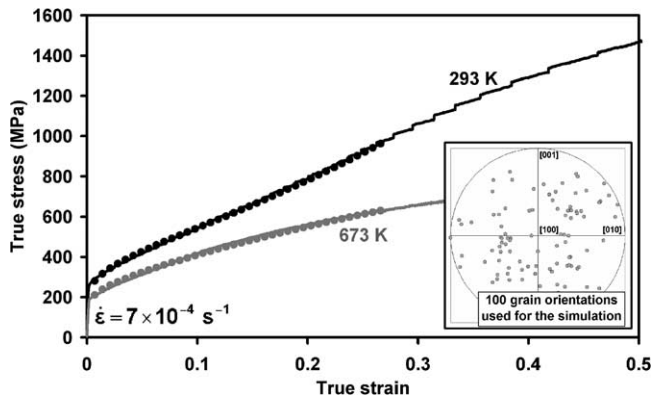


Fig. 1. Experimental (line) and simulated (dot) stress–strain tensile curves for a Fe–22 wt.% Mn–0.6 wt.% C steel at room temperature and at 673 K.

Table 1

Sets of parameters used for the simulation reminding the physical meaning and showing if the parameters are measured (M), estimated (E) or fitted (F) on the experimental curves

	Values	Physical meaning
$\mu$	65 GPa (M)	Shear modulus
$a$	0.361 nm (E)	Lattice parameter
$D$	15.4 $\mu\text{m}$ (M)	Effective grain size
$\rho_0$	$10^{10} \text{ m}^{-2}$ (E)	Initial dislocation density
$\Delta G_0$	96 $\text{kJ mol}^{-1}$ (E)	Activation energy for slip
$V^{\text{a-slip}}$	150 $\text{b}_{110}^3$ (F)	Initial activation volume
$k$	0.03 (F)	Relative hardness of the forest
$f$	2 (F)	Dynamical recovery
$\tau_0$	90 MPa (E)	Friction stress due to carbon
$e$	15 nm (E)	Mean twin thickness
$n$	3 (E)	Microtwin dispersion
$G$	$55 \times 10^3 \text{ m Pa}^{-1}$ (F)	Twinning kinetic

Table 1. The shear modulus was found to be equal elsewhere for both temperatures because of the magnetic transition of the alloy [2,20].

The modeling also predicts the evolution of the deformation microstructure during loading at room temperature. The simulated and experimental reductions of the MFP due to grain and twin boundaries are plotted in Fig. 2.

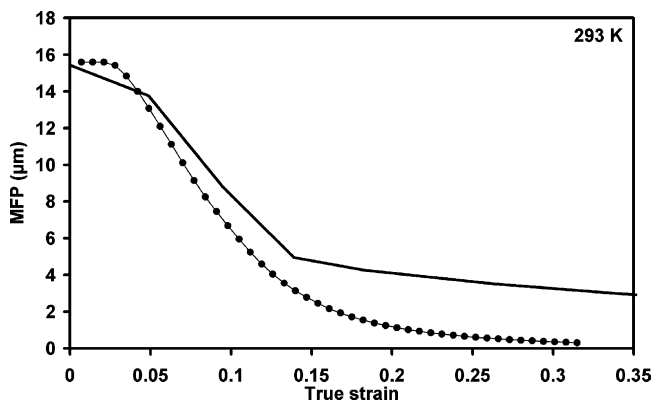


Fig. 2. Evolution of the measured (line) and simulated (dot) mean free path (MFP) for the dislocations due to strong obstacles at room temperature. The MFP is experimentally measured using an intercept count method [9].

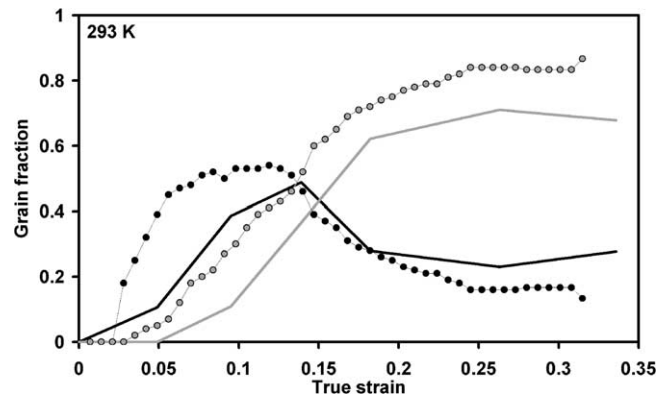


Fig. 3. Evolution of measured (line) and simulated (dot) grain fraction with one (black) or two (light grey) activated twinning systems [9].

In Fig. 3 are plotted the simulated and the measured grain fractions with one or two activated twinning systems during loading. Both simulation results show a good agreement with experimental data. However, the total twinning kinetic do not saturate with strain as expected [4]. This discrepancy can be explained as the twin thickness is kept constant whereas it is supposed to decrease with the MFP of twins [18], and because we do not account for relaxation stress which could hinder twin nucleation.

## 5. Conclusion

The proposed modeling allows to successfully highlight the link between the mechanical and the microstructure properties (TWIP effect) at once. The originality of this model is to account for the typical multiscale organization of twinning and that many parameters could be directly measured or estimated. Moreover, our viscoplastic description explicitly introduces the effect of temperature, which would not have been done using the power-law formalism. Some discrepancies which appear between simulated and expected results are explained.

The simulation is carried out using an easy-to-use homogenization law to deal with the polycrystal. Such model can not account for neither 3D loading, nor grain rotation and relaxation stresses (except with [A]). To fill this gap, our modeling will be introduced into a self-consistent crystal plasticity framework [21,22].

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