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# Modeling of mechanical twinning in a high manganese content austenitic steel

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## Abstract

We propose a 2D simulation of the formation of twins, in correlation with their microstructure observed in a Fe–22 wt.% Mn–0.6 wt.% C austenitic steel deformed at room temperature. TEM observations show that microtwins of a few tens of nanometer thick develop in between grain and twin boundaries, and are stored into stacks of a few tenth of micron wide. We first use a model of the emission of an isolated microtwin, based on the critical stress required to develop successive Shockley dislocation loops along parallel slip planes. As the first loop drags a stacking fault, while the following ones only thicken it, when the critical stress is reached, several dislocations are emitted until the backstress shuts down the source at the equilibrium state. After, the twin thickens stably with the increase of the applied stress. The same model is reproduced to simulate numerically the simultaneous formation of interacting microtwins in a stack. We give a general law correlating the average thickness of the twins with the stacking fault energy, their length, their number and their distance. The thickness is a key parameter in our physically based model presented during this congress.

*Keywords:* TWIP effect; Critical stress; Twin interactions; Stacking fault energy

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## 1. Introduction

At room temperature, the stacking fault energy (SFE) of the studied austenitic Fe–22 wt.% Mn–0.6 wt.% C steel is about  $20 \text{ mJ mol}^{-1}$  [1]. This rather low value promotes mechanical twinning along with strain which is in competition with gliding. Twins are strong obstacles for dislocations as grain boundaries. 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. Thus, the studied alloy shows simultaneously high elongation to fracture (70%) and tensile strength (1200 MPa). The aim of this paper is first to interpret the organization of mechanical twins at different microstructure scales and to qualitatively describe their interactions with dislocations. In the lights of the experimental study, we analyze the twinning process and provide an

easy-to-use tool to predict the thickness of the microtwins derived from the analysis of Friedel [2].

## 2. Characterization of the twinning microstructure

### 2.1. Twinning microstructure at the mesoscopic scale

The experimental procedure has already been described elsewhere [1]. After etching, optical microscopy observations are carried out at the surface of the samples strained at different levels. Fig. 1 shows the evolution of the microstructure with strain. Twins appear as thin bands of a few tenths of micrometer wide. The volume fraction of twins increases obviously with strain, whereas the average distance between them decreases.

The main feature is that one or two systems of parallel twins are observed in each grain. This activation of two systems is sequential. First, one system is activated at the yield point: generated twins develop through the whole grain and are blocked by the grain boundaries. Starting from a given strain, a second system is activated. Twins of the second

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system developed in the interspaces between the twins of the first system and are blocked by them. This process leads to the “ladder-like” pattern of the twin organization observed in Fig. 1. In some rare grains, both systems are activated almost simultaneously, leading to an “ear” pattern, twins of both systems being blocked by twins of the other one.

## 2.2. Twinning microstructure at the microscopic scale

TEM observations show that, at a much smaller scale, the twins previously observed at the mesoscopic scale are actually stacks of microtwins of a few tens of nanometer thick, as already reported by Rémy [3] and Karaman et al. [4,5]. Isolated microtwins, probably not observable in optical microscopy, revealed by etching are also present in the microstructure. Fig. 2(a) shows a TEM micrograph of a sample deformed up to 33%. Only one system is activated and microtwins are organized into stacks indicated by the white arrows. Fig. 3 sums up our understanding of this organization of microtwins.

TEM also confirms the optical microscopy observations: twins cannot pass through grain boundaries and other twins. Fig. 2(b) shows microtwins of a second system (T2) blocked by a microtwin stack of a first system (T1).

The density of defects, i.e. perfect dislocations plus stacking faults bounded by partial dislocations, increases rapidly

with strain. The major gliding activity is located in the not twinned austenite.

The study of all the microtwins in a given grain shows that twins of one system are not only parallel but also produce the same shear. As a consequence, we will be able to discuss the stress acting for twinning in terms of resolved shear stress for different twinning systems, by using Schmidt factors calculated for Shockley Burgers’ vectors.

Concerning the role of the dislocation density on the formation of twins, it is ambivalent: on one hand, dislocation pile-ups provide local stress concentration, strong enough to overcome the critical shear stress for nucleation and the dislocation microstructure also provides potential nucleation sites. On the other hand, forest dislocations introduce obstacles for the thickening of twins.

## 3. Modeling of the twin thickness

One of the most relevant characteristic of twinning is the thickness, which links the volume fraction of twins with their average distance. Very few reliable and statistical measurements of this parameter in previous study are presented in the literature, except [3–5]. To fill this gap, we here propose an easy-to-use formulation which accounts for the most relevant parameters governing twinning in fcc alloys.

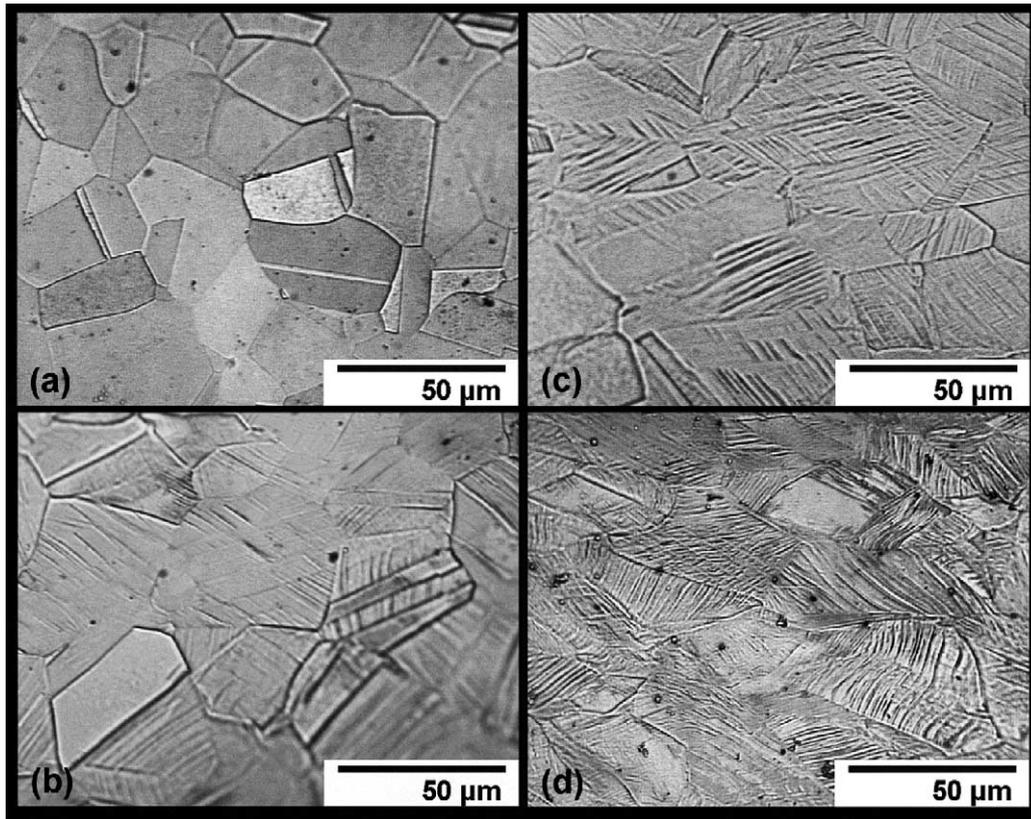


Fig. 1. Optical micrographs after etching to reveal grain boundaries and twins at different strain levels: (a) unstrained, (b) 18%, (c) 26% and (d) 34%. The grain size is about 20  $\mu\text{m}$ . The tensile direction is horizontal.

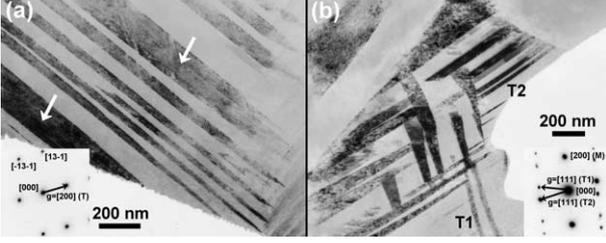


Fig. 2. TEM dark field micrographs after 33% of strain: (a) white arrows indicate parallel stacks of microtwins. Isolated microtwins of the same system are also present and (b) two systems are activated and each system blocks the other.

### 3.1. Modeling of the thickening of an isolated microtwin

The formation of a twin is the result of a glide equal to  $a/6\langle 112 \rangle$ , which is produced by Shockley partials, along successive parallel  $\{111\}$  planes. Friedel [2] has shown that the thickness of a cylindrical twin must evolve linearly with the applied shear stress  $\tau_{\text{applied}}$ . The shape factor  $S$  is given by

$$S = \frac{e}{D} = \frac{2d_{111}}{\mu b} \tau_{\text{applied}} \quad (1)$$

with  $e$  the twin thickness,  $D$  the twin radius,  $d_{111}$  the distance between the  $\{111\}$  planes and  $b$  the Burgers' vector of Shockley partials. This law describes the equilibrium state of the dislocations in the twin front.

The twin tip is blocked on strong obstacles such as grain or twin boundaries [5].  $D$  must then be regarded as half of the mean free path for a twin. For example, for the first system,  $D$  corresponds to half of the grain size.

The weakness of this law is to suppose that even if a low shear stress is applied, twins can nucleate and thicken. We introduce a critical shear stress which corresponds to the stress required for nucleation  $\tau_{\text{nucleation}}$ . It can be expressed as follows [6,7]:

$$\tau_{\text{nucleation}} = \frac{\gamma}{b} + \tau_{\text{loop}} \quad (2)$$

with  $\gamma/b$  the stress required to extend a stacking fault ( $\gamma$  is the SFE) and  $\tau_{\text{loop}}$  the critical stress to expand a dislocation loop. This nucleation stress is only undergone by the very first dislocation of the twin tip since the next ones do not create any stacking fault but only thicken a perfect fcc twin. The stress required to emit and move these following dislocations is only equal to  $\tau_{\text{loop}}$ .

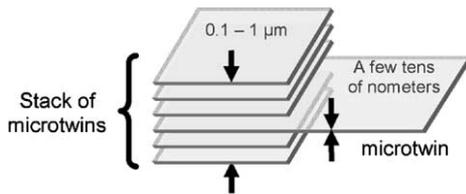


Fig. 3. Order of magnitude and understandings of the microtwin organization into stacks.

The twinning mechanism can be decomposed into two stages. First, the applied shear stress reaches the critical nucleation stress, the first dislocation is emitted from the source, and several dislocations follow, since their critical emission stress is lower. This process stops when the backstress produced by the dislocations blocked by the obstacle becomes higher than  $\tau_{\text{loop}}$ . As a consequence, a numerous dislocations are emitted instantaneously at  $\tau_{\text{applied}} = \tau_{\text{nucleation}}$ . This behavior explains the rapid development of twins [2,8] and the high level of acoustic emission recorded when mechanical twinning occurs during a tensile test [1].

The equilibrium state of the twin is calculated by shifting Friedel's result by  $\tau_{\text{loop}}$ :

$$S = \frac{e}{D} = \frac{2d_{111}}{\mu b} (\tau_{\text{applied}} - \tau_{\text{loop}}) \quad (3)$$

Since these dislocations have been emitted for  $\tau_{\text{applied}} = \tau_{\text{nucleation}}$ . The thickness of the twin is at least equal to

$$e_{\text{min}} = \frac{2d_{111}}{\mu b} \left( \frac{\gamma}{b} \right) D \quad (4)$$

The number of emitted dislocations  $N_{\text{min}}$  during this first stage is

$$N_{\text{min}} = \frac{e_{\text{min}}}{d_{111}} = \frac{2}{\mu b} \left( \frac{\gamma}{b} \right) D \quad (5)$$

The second stage of the twinning process consists in a thickening. If  $\tau_{\text{applied}}$  increases ( $\tau_{\text{applied}} > \tau_{\text{nucleation}}$ ), new dislocations are emitted by the nucleus. The equilibrium state is still defined by the linear law (Eq. (3)). This two-stage process is represented in Fig. 4. The significant parameters defined by Eqs. (2) and (5) are indicated.

### 3.2. Discussion

Friedel's model assumes a cylindrical shape of the twin. But, some of the dislocations in the twin tip do not reach the obstacle, as observed in Marcinkowski et al. numerical analysis [9,10]. They reach their equilibrium position before

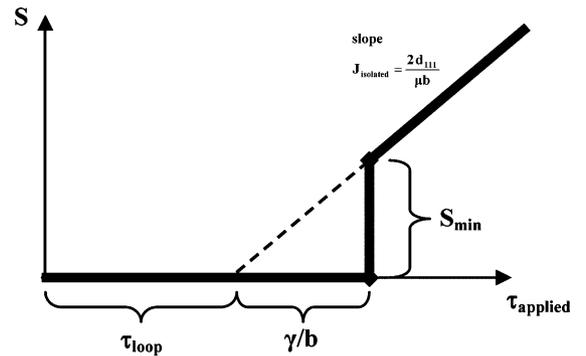


Fig. 4. Evolution of the twin shape factor with the stress. The thick line shows the equilibrium state of the twin.

the obstacle, due to the backstress of the previously emitted dislocations and form a pile-up leading to a lenticular shape. We also observe this experimentally. This is taken into account in our modeling by dislocations presented in the next section, contrary to Müllner's interpretation of twinning [11].

In our alloy, the lattice is highly deformed by dislocation gliding which leads to a high density of forest obstacles. In such conditions, the first stage of the formation of a microtwin, where numerous partials act collectively to glide through the forest, can occur. On the other hand, the regular growth along with an increase of the applied stress in the second stage, involving individual dislocations, may be hindered and probably inhibited [12]. Consequently, modeling twinning in our alloy may be done with little error, by considering microtwins of the minimal thickness given by Eq. (4).

As previously described, two twinning systems are activated sequentially. When the first twinning system is activated, twins develop through the whole grain. The distance  $D$  is then equal to the grain size. We assume that twins nucleate at the grain boundary by heterogeneous nucleation [1,6]. Since twin boundaries are strong obstacles, twins of the second system develop from one twin boundary of the first system to another. The distance  $D$  is then the distance between twins of the first system, much smaller than the grain size. Consequently, in agreement with Eq. (4), twins of the second system must be much thinner than the twins of the first one.

### 3.3. 2D simulation

The linear law equation (3) is easy-to-use for an isolated twin, but cannot be used to describe complex interactions between multiple microtwins in a stack. We develop a simulation which first model the equilibrium of the tip of a single twin under an applied stress, at the scale of 2D elastic interactions between straight dislocations, as done by Jin and Bieler [13]. The nucleus emits free partial dislocations as previously discussed.

The results show a good agreement with the previous analytical modeling. The evolution of the shape factor follows a linear law but the slope  $J_{\text{isolated}}$  is reassessed numerically ( $J_{\text{isolated}} = 7.1 \times 10^{-5} \text{ MPa}^{-1}$  instead of  $J_{\text{isolated}} = 4.4 \times 10^{-5} \text{ MPa}^{-1}$  given by (3)). The dislocations of the twin tip show the same behavior as proposed by Mitchell and Hirth [9]. The formation of a pile-up instead of a cylindrical wall explains the discrepancy between the analytical and the simulated slope  $J_{\text{isolated}}$ .

We calculate the stress field around such a spread pile-up and define the zone where the backstress is higher than  $\tau_{\text{loop}}$ . The width of this zone is of the order of a few tenths of the twin length (grain size), and does not depend on the twin thickness. This means that once a microtwin is formed, others of the same system may develop over this distance from the first one. This is not in agreement with the organization

of microtwins into stacks previously discussed, unless they are created simultaneously.

### 3.4. Interacting microtwins

The stack is modeled by introducing  $n$  co-planar microtwin sources separated by a constant distance  $\lambda$ . Each twin nucleus is placed at the same distance  $D$  from an obstacle and all the nuclei are activated simultaneously. After compiling numerous simulation results for different sets of  $(n, \lambda)$ , we obtain that the mean shape factor of the microtwins in a stack still follows a linear law and that the slope fits the following empirical law:

$$J_{\text{mean}}(\lambda, n, D) = J_{\text{isolated}} \left( \frac{1 - e^{-\lambda/D}}{1 - e^{-n\lambda/D}} \right) \quad (6)$$

Assuming that no thickening stage occurs, Eqs. (4) and (6) give the twin thickness:

$$e_{\text{mean}} = J_{\text{isolated}} D \left( \frac{1 - e^{-\lambda/D}}{1 - e^{-n\lambda/D}} \right) \frac{\gamma}{b} \quad (7)$$

with  $J_{\text{isolated}} = 7.1 \times 10^{-5} \text{ MPa}^{-1}$  according to the simulation for our alloy.

The measured mean thickness of the microtwins in our steel is about 30–60 nm. This measure is problematical in our material in so far as the density of dislocations and stacking faults is very high near the twin boundaries. In our case,  $D = 15.6 \mu\text{m}$ ,  $b = 1.47 \text{ \AA}$ ,  $\gamma = 20 \text{ mJ m}^{-2}$  which leads to  $e = 90 \text{ nm}$  for an isolated twin and  $e = 20 \text{ nm}$  for a stack containing five microtwins separated by 50 nm. This simulation result is consistent with our measurements and previous studies in the literature [4,5].

## 4. Conclusions

The multiscale study of the deformation microstructure of an austenitic Fe–22 wt.% Mn–0.6 wt.% C steel at room temperature shows that:

- mechanical twinning and dislocation gliding enter in competition and closely interact in each grain,
- two twinning systems are sequentially activated in most grains,
- twin and grain boundaries are strong obstacles for twins, microtwins of a few tens of nanometers thick are generally gathered into stacks of a few tenths of micrometer thick.

We model the development of interacting microtwins at the scale of the elastic interactions between dislocations. By reflecting our understanding of microtwinning, our modeling is able to predict some characteristics of the microstructure such as the twin thickness and the stress field around twins.

The twinning process can be decomposed into two sequential stages. First, the twin tip moves from the nucleus to the next strong obstacle (grain or twin boundary) at a given critical stress, and second, the twin thickens when the applied stress increases. This thickening depends linearly on the applied shear stress. We provide an analytical formula for the prevision of the thickness of parallel twins, which only depends on physical and measurable parameters. In particular the thickness is shown to scale like the grain size and the SFE. The given orders of magnitude are in good agreement with experimental results.

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