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# On the strain hardening and texture evolution in high manganese steels: Experiments and numerical investigation <sup>☆</sup>



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## ABSTRACT

We present a systematic investigation on the strain hardening and texture evolution in high manganese steels where twinning induced plasticity (TWIP) plays a significant role for the materials' plastic deformation. Motivated by the stress–strain behavior of typical TWIP steels with compositions of Fe, Mn, and C, we develop a mechanistic model to explain the strain-hardening in crystals where deformation twinning dominates the plastic deformation. The classical single crystal plasticity model accounting for both dislocation slip and deformation twinning are then employed to simulate the plastic deformation in polycrystalline TWIP steels. While only deformation twinning is activated for plasticity, the simulations with samples composed of voronoi grains cannot fully capture the texture evolution of the TWIP steel. By including both twinning deformation and dislocation slip, the model is able to capture both the stress–strain behaviors and the texture evolution in Fe–Mn–C TWIP steel in different boundary-value problems. Further analysis on the strain contributions by both mechanisms suggests that deformation twinning plays the dominant role at the initial stage of plasticity in TWIP steels, and dislocation slip becomes increasingly important at large strains.

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## 1. Introduction

The high ultimate strength, combined with a high hardening modulus to resist deformation localization in the twinning induced plasticity (TWIP) steels, stimulate broad interests from both academic society and industries. For example, Fe–Mn–Si–Al and Fe–Mn–C austenitic TWIP steels have been proposed to many applications (Grässel et al., 2000) where high strength and/or light weight materials are desired for lower energy consumption and further enhancement in safety, which is of paramount importance in the automotive industry (Liu et al., 2012). For example, the ultimate strength over density ratio of TWIP steels is comparable to that of nanocrystalline magnesium (Wei and Anand, 2007). Typically, the 0.2% yield strengths of TWIP steels are in the range of 350–500 MPa, which are at the same level of several conventional high strength steels including dual-phase (DP) steels and transformation-induced plasticity (TRIP) steels (Bouaziz et al., 2011a, 2011b; Krauss, 1990; Yoo et al., 2009; Zavattieri et al., 2009). Following the initial yielding, TWIP steels harden at a nearly constant

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modulus on the order of 1 GPa (Allain et al., 2008; Bouaziz, 2012; Bouaziz et al., 2010, 2008; Bouaziz and Guelton, 2001; Chen et al., 2007; Ding et al., 2011; Idrissi et al., 2010b; Jin and Lee, 2009; Liang et al., 2009; Sevillano, 2009; Shiekhelsouk et al., 2009). Due to the high strain hardening, TWIP steels can attain an elongation about 60–95%, and the corresponding ultimate strength is about 800 MPa to 1.8 GPa (Allain, 2002; Allain et al., 2002; Bayraktar et al., 2004; Chen et al., 2007; Dastur and Leslie, 1981; Frommeyer et al., 2003; Grässel et al., 2000; Huang et al., 2006; Kim et al., 2009; Lai and Wan, 1989; Mi et al., 2005, 2012; Vercammen, 2004). The diagram given in Fig. 1 summarizes the mechanics properties of several steels and other metallic materials of current interest, among which TWIP steels owe the most promising combination of strength and deformability.

The attractive properties in TWIP steels are attributed to the activation of twinning during their plastic deformation. At room temperature, deformation twinning is not regarded as the primary plastic carrier in conventional face centered cubic (FCC) metals because their stacking fault energy (SFE) is relatively high. It is reported that low intrinsic stacking fault energy  $\gamma_{sf}$  (below approximately 20 mJ/m<sup>2</sup>) favors the  $\gamma$  (FCC phase) to  $\epsilon$  (hexagonal close-packed, HCP phase) transformation in TWIP steels; while  $\gamma_{sf} > 20$  mJ/m<sup>2</sup>, this phase transformation is rarely observed (Sato et al., 1989). When  $\gamma_{sf}$  is too high, motion of complete dislocations takes over and becomes the primary plastic deformation mechanism. Such a transition can be readily explained if the nucleation of  $a/6\langle 112 \rangle$  Shockley partial dislocations and  $a/2\langle 110 \rangle$  complete dislocations are the controlling factors for the competition between deformation twinning and dislocation glide. The critical resolved shear stress (CRSS)  $\tau_{crss}$  for the nucleation of an  $a/6\langle 112 \rangle$  Shockley partial dislocation is about  $\tau_{crss} = \gamma_{sf}/b + \alpha Gb/3d$  (Asaro et al., 2003; Asaro and Suresh, 2005; Wei et al., 2006; Zhu et al., 2005), while the CRSS  $\tau_{crss}$  for the nucleation of a complete dislocation approximates to  $\beta Gb/d$ , where  $b$  is the Burgers vector,  $G$  is the shear modulus,  $d$  is the grain size, and  $\alpha$  and  $\beta$  are coefficients on the order of unit. The expressions for  $\tau_{crss}$  indicate that materials with higher SFE tend to nucleate complete dislocations. That is to say, the SFE of FCC austenite needs to be in the right range, neither too low nor too high, in order to promote deformation twinning while the material is deforming at a certain range of temperatures and strain rates. Current understanding on the roles of manganese and carbon (or its alternatives) in TWIP steel enables us to tune the composition of the materials and achieve the suitable SFE to promote deformation twinning (Allain et al., 2010; Br ux et al., 2002; Curtze and Kuokkala, 2010; Curtze et al., 2011; Dumay et al., 2008; Idrissi et al., 2010a, 2009; Jeong et al., 2012; Jin and Lee, 2012; Lee et al., 2010; Park et al., 2010; Saeed-Akbari et al., 2011; Wang et al., 2010; Yoo and Park, 2008). It is worth pointing out that appropriate SFE is necessary but by no means a sufficient condition for twinning (Bouaziz et al., 2011a; Meyers et al., 2001). As commented by Christian and Mahajan (1995), loading modes, temperature, residual strain, grain size, and strain-rate all influence the activation of deformation twinning.

From the crystallographic aspect, motion of a complete dislocation gives rise to shear displacement of a portion of the crystal over another and leaves the lattice virtually unchanged. In contrast, shear displacement induced by a Shockley partial dislocation is only a fraction of the inter-atomic spacing. During twinning, the nucleation and gliding of several leading partials in successive planes result in mirror image lattice reorientations across the boundary. Now in addition to the initial crystallographic texture characteristics of TWIP steels resulted from rolling processing, deformation twinning further alters the texture dramatically. The reorientation induced by twinning brings exceptional yet unique characteristics in crystalline materials. For example, it is evident that the consequently formed mirror planes are effective barriers to dislocation slips inclined to those planes (Li et al., 2010). It hence enhances the strength of the material as deformation proceeds. As a result,

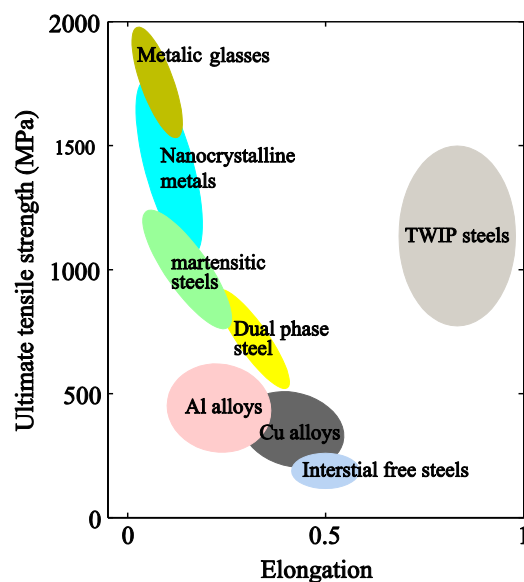
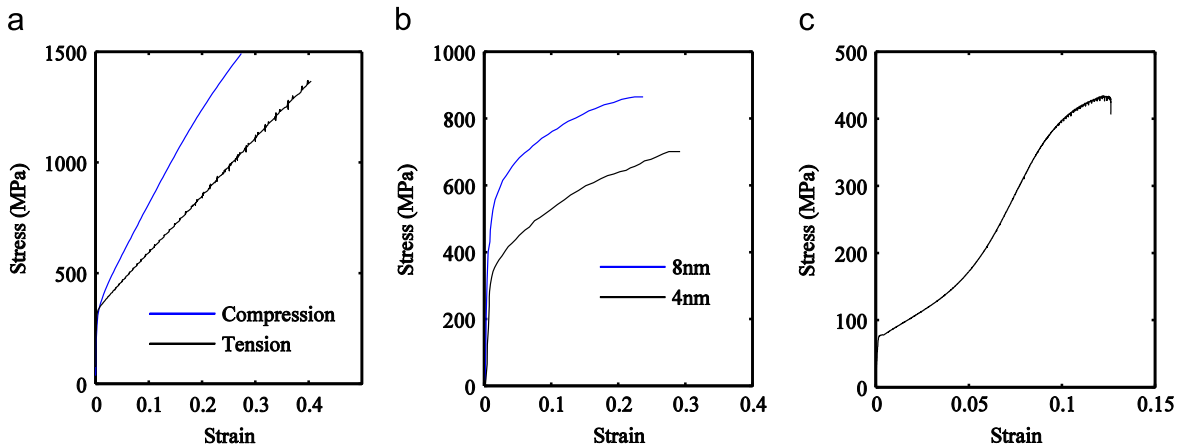


Fig. 1. Illustration to show the ultimate tensile strength versus elongation for several conventional metals, as well as metallic glasses and nanocrystalline metals. TWIP steels owe both high strength and large tensile elongation.



**Fig. 2.** Strain hardening in crystalline metals where twinning plays a significant role in plastic deformation. (a) Compressive and tensile stress–strain curves for a high-manganese steel (Fe23.84Mn0.61C, wt%); (b) the stress–strain curves (replotted) for nano-twinned crystalline Cu samples with average twin thicknesses of 4 nm and 8 nm (Lu et al., 2009). Deformation twinning is regarded as one of the primary plastic deformation mechanisms in such samples with preexisting twins; (c) Compressive stress–strain curve for magnesium alloy AZ31B.

**Table 1**

Chemical compositions (in weight percentage, wt%) of the FeMnC TWIP steel investigated in this study.

Name	Fe	Mn	C
Fe23.84Mn0.61C	0.7554	0.2384	0.0061

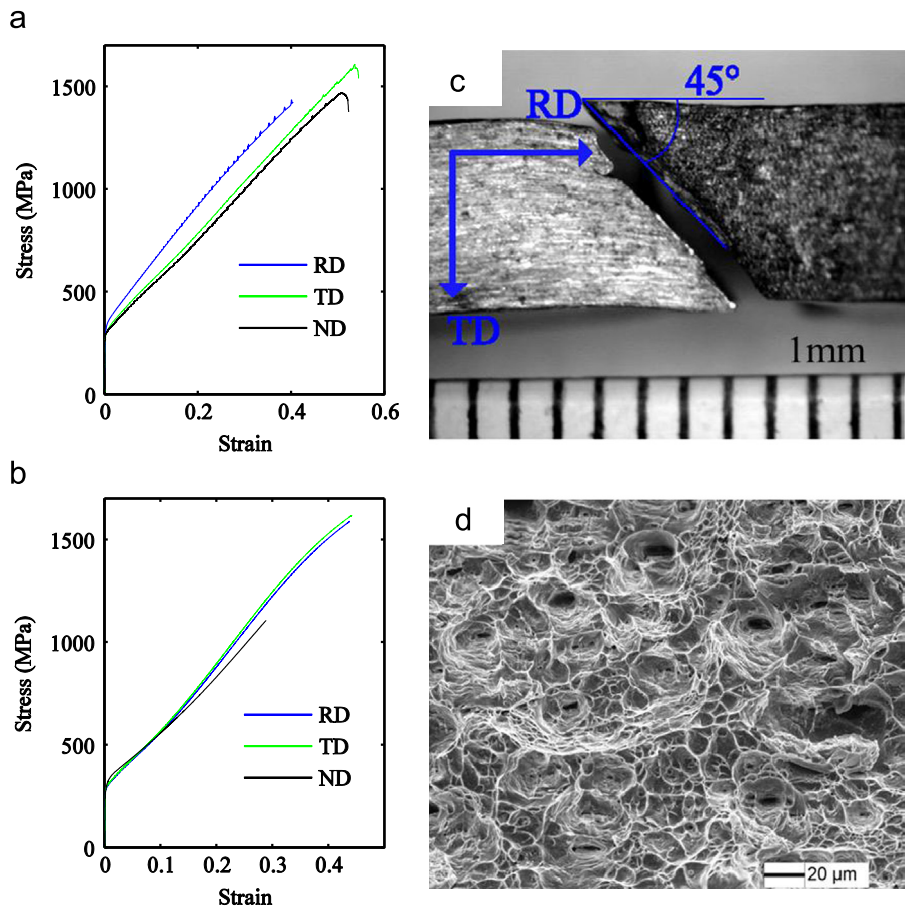
those materials where deformation twinning plays a significant role in plasticity commonly exhibit high strain hardening. Fig. 2 presents several typical examples of crystalline metals where deformation twinning plays a crucial role for their plastic deformation.

In order to understand the mechanisms accounting for the enormous strain hardening in TWIP steels, there is a pressing need to reveal the correlation between texture evolution and strain hardening by deformation twinning. In addition, while it is generally accepted that mechanical twinning is competitive to dislocation motion in TWIP steels, the role played by each mechanism at different stages of deformation is hard to abstract from experiments, due to the factor that current experimental observations are usually carried out on post-mortem samples. Last but not least, the remarkable deformability in TWIP steels is desired in industrial plastic forming (Chung et al., 2011; Cooman et al., 2011, 2005; Scott et al., 2006), and it is now important to supply reliable simulating tools for the manufacturing processing for TWIP steels, while using the materials to make complex parts by stamping. With the motivations given above, here we conduct both experimental characterizations and numerical simulations, in hope to reveal the hardening mechanisms and the texture evolution in TWIP steels during plastic deformation.

## 2. Experimental results

Since the pioneering work of Hadfield (Adler et al., 1986; Dastur and Leslie, 1981; Karaman et al., 2000; Raghavan et al., 1969), steels with fully austenitic microstructures but different compositions have been made. Two categories of the family, which were named by their characteristics in plastic deformation, TRIP and TWIP steels, have been intensively investigated in the last decade. It is generally accepted that TWIP steels have high manganese content in the range of 12–30 wt%. Here we choose one TWIP steels with elements of Fe, Mn, and C for our investigation. For simplicity, we use FeMnC as the name of the TWIP steel in what follows. In Table 1, we show the specific chemical compositions for the FeMnC TWIP steel in the present study.

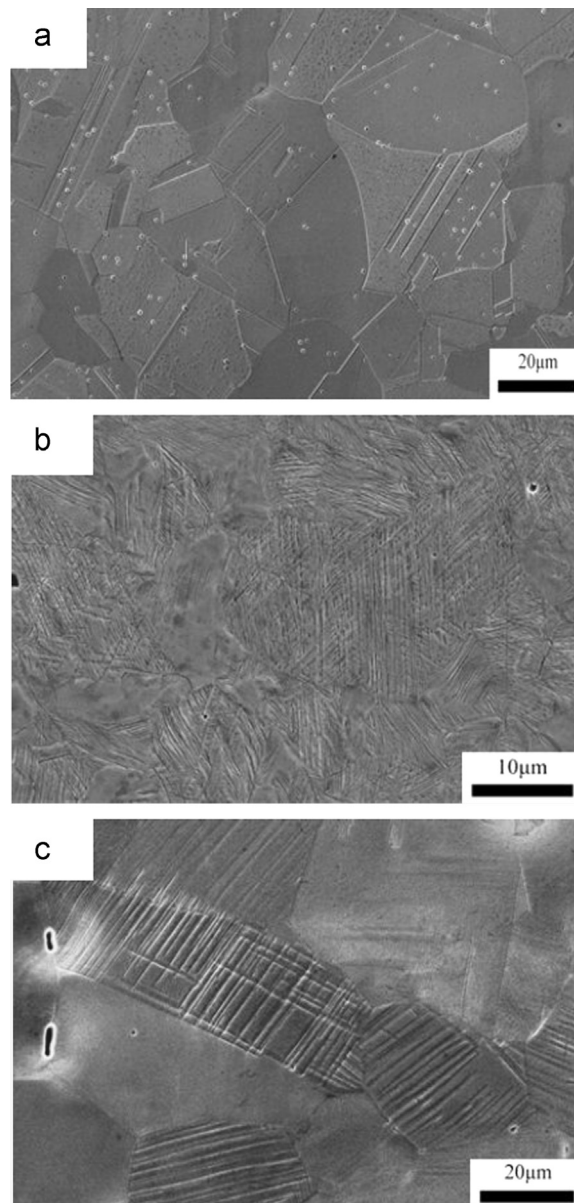
The elements were melted in vacuum induction furnace and protected with Ar gas. We then cast the molten steel to flat ingot. Rolling is conducted at the initial rolling temperature of 1050 °C, and at the finishing temperature of 975 °C. The final hot rolling plate is about 26.0 mm thick. The plates are then gone through air cooling. After cooling, we cut specimens from those plates for further mechanical tests. For convenience, we use the coordinate system defined by the rolling direction (RD), the transverse direction (TD), and the normal direction (ND) to characterize the tested samples. Fig. 3a shows the tensile stress–strain behavior for the TWIP steel at low strain rates. True stress–strain responses in the RD, TD and ND show slight difference, which is consistency with the previous observation that there is weak initial texture (Bouaziz et al., 2011a). Corresponding compressive stress–strain responses in the three directions are given in Fig. 3b.



**Fig. 3.** The quasi-static stress–strain response of FeMnC. (a) Tensile stress–strain curves in the rolling direction (RD), the transverse direction (TD), and the normal direction (ND). (b) Compressive stress–strain curves in the three directions. (c) Macroscopic fracture patterns for TWIP steels with tensile loading in the RD direction. (d) Fractographic examination to show the ductile feature of the fracture surfaces in TWIP steels, where large amount of bird nest type dimples are seen.

Due to the extraordinary deformability for TWIP steels, none of the samples subjected to compression were fractured after the applied deformation. The macroscopic failure pattern of the tensile samples in the RD is given in Fig. 3c. The fracture results from typical shear failure, with the shear angle between the failure plane and the loading axis about  $45^\circ$ . Large amount of bird nest type dimples left by severe plastic flow are seen in the fractographic observation, as evidently observed in the scanning electron microscope (SEM) pictures shown in Fig. 3d. In addition to the fractographic observation presented in Fig. 3, we show in Fig. 4 the characteristic of microscopic structures after different deformation modes. As a comparison, the initial microstructure of the FeMnC TWIP steel is given in Fig. 4a. There is perceivable amount of preexisting annealing twins in the material. After quasi-static tension, enormous amount of lenticular twins and slip lines in austenitic grains are formed, see Fig. 4b. The same type of deformation twinning is seen in samples after quasi-static compression, as shown in Fig. 4c. Inspired by the large amount of twinning and dislocation activities, we will try to quantify the activated deformation twinning and dislocation slips by measuring the orientation density of the materials before and after deformation.

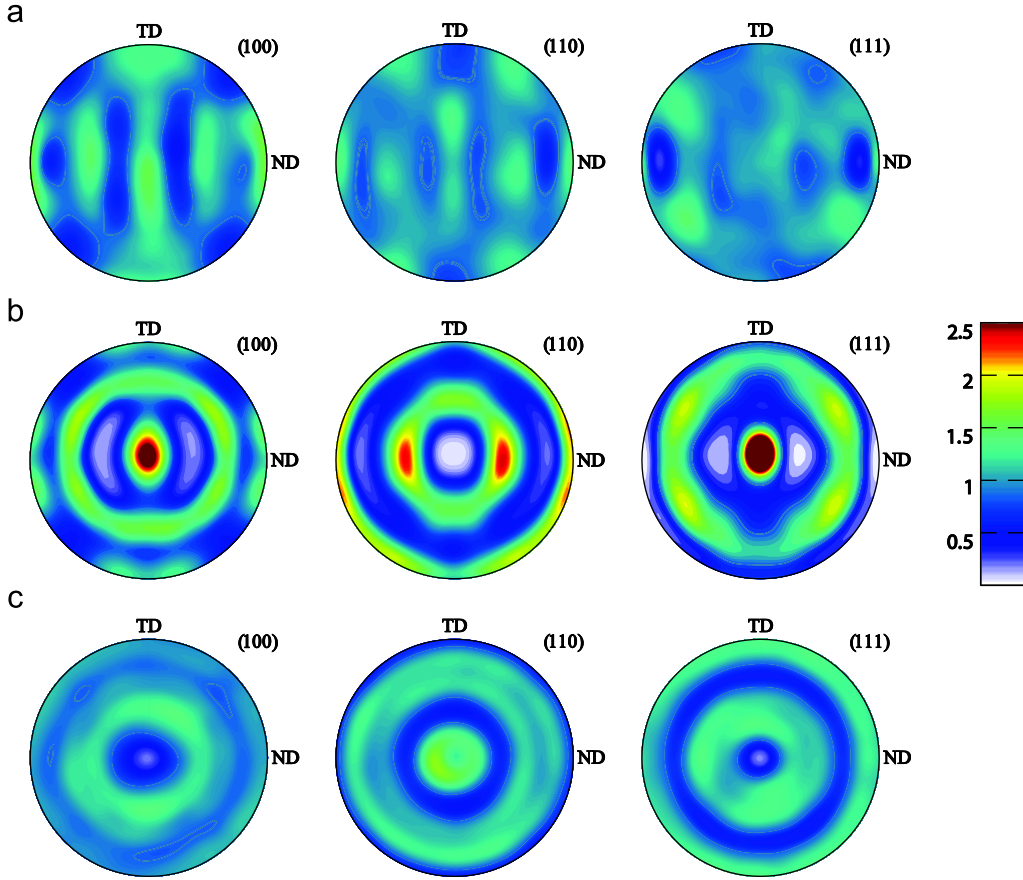
We show in Fig. 5a the initial texture in FeMnC in the rolling direction. For here and in what follows, all pole figures are equal-area projections of the specified crystallographic planes. The main components of texture in TWIP steels are cubic-type texture  $\{001\} \langle 100 \rangle$ , rotated brass-type texture  $\{110\} \langle 111 \rangle$  and the E-type texture  $\{111\} \langle 110 \rangle$  (Lü et al., 2010; Vercammen et al., 2004). The intensity of texture in the TWIP steel, however, is rather weak. This observation is consistent with existing experiments (Bracke et al., 2009; Lü et al., 2011; Saleh et al., 2011). After tension, the primary orientations of the TWIP steel become the cubic-type texture  $\{001\} \langle 100 \rangle$  and the rotated brass-type texture  $\{110\} \langle 111 \rangle$  (see Fig. 5b). Given grains from  $\langle 111 \rangle$  orientation are adequate for twinning whereas  $\langle 100 \rangle$  fiber orientation are more suitable for slip, the final texture reflects a combination impact of twinning and slip (Barbier et al., 2012, 2009a, 2009b; Gutierrez-Urrutia et al., 2010; Meng et al., 2007; Yang et al., 2006). In contrast, after quasi-static compression, the main components of textures are the rotation Goss-type texture  $\{110\} \langle 110 \rangle$ , Goss/Brass type texture (in between the Goss type texture and the brass-type texture), as well as Goss twin-type texture  $\{113\} \langle 332 \rangle$  (see Fig. 5c).



**Fig. 4.** Scanning electron microscopy of TWIP steels to show microstructures at different stages of deformation. (a) Initial sample with average grain size about 35  $\mu\text{m}$ . (b) Microstructures after quasi-static tension (strain rate:  $10^{-3} \text{ s}^{-1}$ , tensile strain about 56%). (c) Deformation pattern after quasi-static compression (strain rate:  $10^{-3} \text{ s}^{-1}$ , compressive strain about 43%).

### 3. A mechanistic model for strain hardening by twin thickening

As seen from the microstructures in the deformed samples, there exists large amount of deformation twinning in the TWIP steel after deformation. Now we aim to develop a simple model to capture the strain hardening seen in the stress–strain curves in Fig. 3. By assuming that plasticity is dominated by deformation twinning, we see several scenarios which could result in strengthening in TWIP steels. (a) Dislocation pileup by deformation twinning: from the perspective based on the interaction between dislocations and grain boundaries, a deformation twin usually results in the formation of two dislocation walls at the two ends of a twinned lenticle. If those dislocations are not absorbed by the GBs, they will contribute to strengthening. (b) Twin boundary as barriers to dislocations or secondary twins: it is well known that by increasing grain boundaries (GBs) numbers as grain sizes reduce; we could achieve substantial increasing in strength in crystalline metals (Li et al., 2010; Lu et al., 2009, 2004). The formation of low energy and coherent twin boundaries (TBs) supplies a desired strengthening mechanism in polycrystalline metals (Allain et al., 2004a, 2004b, 2004c; Bouaziz and Guelton, 2001; Brück et al., 2002). (c) Depletion of easy twinning regions: if twinning is the only plastic deformation in a polycrystalline metal, the gradual depletion of easy-to-be-twinned grains while straining hardens the materials as well.



**Fig. 5.** Texture of FeMnC TWIP steel in RD at different status. (a) Initial texture in three different crystallographic planes. (b) Texture after 56% tensile strain. (c) Texture after 43% compression strain.

Here we present a tentative theoretical analysis regarding how deformation twinning can give rise to nearly constant strain hardening modulus. We start with using the free energy  $F$  associated with the nucleation of a twin lamina with width  $\lambda$  in a grain with size  $d$  (Wei, 2011a):

$$F = \left[ \frac{\pi}{8} \frac{2-\nu}{1-\nu} \frac{\lambda}{d} G(e^T)^2 - (\tau - \tau_1)e^T \right] V + 2\gamma_{sf}S, \quad (1)$$

where  $G$  is the shear modulus,  $\nu$  is Poisson's ratio,  $V = \pi d^2 \lambda / 4$  and  $S = \pi d^2 / 4$ ,  $e^T$  is the shear strain associated with twinning/de-twinning,  $\gamma_{sf}$  is the twin-boundary energy, and  $\tau$  and  $\tau_1$  are the applied shear stress and the lattice resistance, respectively. This energy term is derived by treating the twin lamina as an inclusion with uniform shearing (Eshelby, 1957). By applying the above equation to dislocation-mediated twinning in an incremental manner, we obtain the free energy associated with the thinnest twins as

$$\frac{F}{V} = \frac{\pi}{8} \frac{2-\nu}{1-\nu} \frac{3d_{(111)}}{d} G(e^T)^2 - (\tau - \tau_1)e^T + \frac{2\gamma_{sf}}{3d_{(111)}}. \quad (2)$$

here  $d_{(111)}$  is the space of between two neighboring (111) planes. It requires at least three layers of (111) atomic planes to define a twin fault (Mahajan and Chin, 1973). With  $F \leq 0$  for successful nucleation of a twin embryo, we obtain the corresponding critical stress to be

$$\tau = \tau_1 + \frac{\pi}{8} \frac{2-\nu}{1-\nu} \frac{3d_{(111)}}{d} G e^T + \frac{2\gamma_{sf}}{3e^T d_{(111)}}. \quad (3)$$

Assuming that the dislocations are not being absorbed by grain boundaries, after the twinning of  $n$  successive layers, the free energy change to add another atomic plane to the twinned region would be

$$\Delta F = F(n+1) - F(n) = \left[ \frac{\pi}{8} \frac{2-\nu}{1-\nu} \frac{(2n+1)d_{(111)}}{d} G(e^T)^2 - (\tau - \tau_1)e^T \right] \frac{\pi d^2}{4} d_{(111)}. \quad (4)$$

**Table 2**

Material parameters for nanotwinned Cu (ntwin-Cu) and FeMnC. When deformation twinning is the dominant mechanism for plasticity, the predicted hardening modulus  $H$  using Eq. (7) is close to the experimental measurement  $H_{exp}$ .

	$G$ (GPa)	$\nu$	$\gamma_{sf}$ (mJ/m <sup>2</sup> )	$e^T$	$d_{(111)}$ (nm)	$b$ (nm)	$\lambda$ (nm)	$d$ ( $\mu$ m)	$H$ (GPa)	$H_{exp}$ (GPa)
ntwin-Cu	40	0.34	45	0.707	0.156	0.148	$\sim 5$	0.5	1.8	1.5–2.5
FeMnC	65	0.3	20	0.707	0.208	0.197	$\sim 100$	10	2.7	2–5

By applying  $\Delta F \leq 0$ , we yield the critical stress for the initiation of dislocation motion for the  $(n+1)$ -th layer to be

$$\tau_{flow} = \frac{\pi 2-\nu(n+1)d_{(111)}}{4 1-\nu d} Ge^T + \tau_l + \frac{\pi 2-\nu d_{(111)}}{8 1-\nu d} Ge^T. \quad (5)$$

Therefore, if we assume the dislocations are not absorbed by the GB, the flow stress would steadily increase with each additional layer of twinning. The hardening by the growth of twins can be obtained based on Eq. (5) by assuming that deformation twinning is the only plastic carrier. For a twinned region with thickness  $\lambda$ , further thickening by emission of one partial dislocation gives a plastic strain increment  $\epsilon_0 = b/\lambda$  (Wei, 2011a). With Eq. (5), the hardening by twin growth is

$$\frac{d\tau_{flow}}{d\epsilon} \approx \frac{\tau_{flow}(n+1) - \tau_{flow}(n)}{\epsilon_0} = \frac{\pi 2-\nu d_{(111)}}{4 1-\nu d} Ge^T \frac{1}{\epsilon_0}. \quad (6)$$

By taking into account the influence of crystallographic orientations, the hardening modulus by twin growth can be rewritten as

$$H = \beta_T \frac{d\tau_{flow}}{d\epsilon} = \beta_T \frac{\pi 2-\nu d_{(111)} \lambda}{4 1-\nu b d} Ge^T. \quad (7)$$

where  $\beta_T=3$  is the Taylor factor. We show in Table 2 the hardening moduli predicted by the theoretical analysis for two typical materials where deformation twinning is regarded as their primary carrier for plasticity. The theoretical results for the two materials match reasonably well with experimental measurements. Eq. (7) also implies that twinning dominated plasticity may give rise to higher strain hardening modulus as twins are thickening ( $\lambda$  increases) as plasticity accumulates, which is in qualitative agreement with experiment observations for metals where deformation twinning is their primary deformation mechanism for plasticity (see Fig. 2c and Fig. 3a and b).

#### 4. Crystal plasticity model for twinning and dislocation slip

In addition to the theoretical analysis, we are interested in exploring the deformation in TWIP steel by physically rooted constitutive models. We employ the classical framework of rate-independent single-crystal plasticity (Asaro and Needleman, 1985; Dancette et al., 2012; Kalidindi et al., 1992; Roters et al., 2010) to model plasticity by dislocation slip. There also exists pioneering work to model deformation twinning in the continuum mechanics frame (Kochmann and Le, 2009; Staroselsky and Anand, 1998; Staroselsky, 1998). Staroselsky and Anand put forward a crystal plasticity model for FCC materials by taking both slip and twinning accommodated plasticity into account (Staroselsky and Anand, 1998); Fernández et al. improved the model by considering cross-hardening between slip and twinning systems (Fernández et al., 2011). The influence of pre-existing twins to the ductility and strength behavior of materials has also been investigated by Jérusalem et al. (2008) using finite-element based crystal plasticity simulations; Proust et al. implemented a meso-scale composite grain model to understand the texture, twinning and hardening evolution of pure Zr (Proust et al., 2007). Here we adopt the single crystal scheme developed by Staroselsky and Anand (Staroselsky and Anand, 1998; Staroselsky, 1998). For completeness, we repeat here part of the key ingredients. In such framework, the deformation gradient  $\mathbf{F}$  is decomposed into elastic ( $\mathbf{F}^e$ ) and plastic ( $\mathbf{F}^p$ ) parts as

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p, \quad (8)$$

with  $\det(\mathbf{F}^e) > 0$  and  $\det(\mathbf{F}^p) = 1$ . Plastic flow takes place through both dislocation slip and deformation twinning in prescribed crystallographic slip/twinning systems. Here, we use integer  $i$  to label crystal slip systems and integer  $\alpha$  to label crystal twin systems. At the initial configuration, each slip system is defined by a slip/twinning direction  $\mathbf{m}_0$  and a slip/twinning-plane normal  $\mathbf{n}_0$ . The Green elastic strain measure  $\mathbf{E}^e$  and the symmetric second Piola–Kirchhoff stress tensor  $\mathbf{T}$  are hence defined respectively as

$$\mathbf{E}^e \equiv (1/2)(\mathbf{F}^{eT} \mathbf{F}^e - \mathbf{1}) \text{ and } \mathbf{T} \equiv \mathbf{C} \mathbf{E}^e, \quad (9)$$

where the superscript ‘T’ stands for the transpose of a tensor and  $\mathbf{C}$  is the fourth order tensor of elastic moduli. The resolved shear stress  $\tau$  on the slip/twinning system  $(\mathbf{m}_0, \mathbf{n}_0)$  is calculated as

$$\tau = (\mathbf{F}^{eT} \mathbf{F}^e \mathbf{T}) \cdot (\mathbf{m}_0 \otimes \mathbf{n}_0). \quad (10)$$

The evolution of plastic deformation gradient, on multiple  $i/\alpha$ -th slip/twin systems, is given as

$$\mathbf{F}^p = 1 + \sum_i \Delta\gamma^i \mathbf{S}_0^i + \sum_\alpha \Delta\gamma^\alpha \mathbf{S}_0^\alpha, \mathbf{S}_0^i \equiv \mathbf{m}_0^i \otimes \mathbf{n}_0^i \text{ and } \mathbf{S}_0^\alpha \equiv \mathbf{m}_0^\alpha \otimes \mathbf{n}_0^\alpha \quad (11)$$

where  $\mathbf{S}_0^i$  is the Schmid tensor for the  $i$ -th slip system, and  $\mathbf{S}_0^\alpha$  is the Schmid tensor for the  $\alpha$ -th twin system.  $\Delta\gamma$  is the incremental shear due to slip/twinning, which is determined by using the consistency condition in rate-independent plasticity scheme given the resolved shear stress  $\tau$  and the resistance  $S$  on the slip/twinning system.

One of the major uncertainties is how to capture the slip/twin hardening. Simple phenomenological models for the evolution of  $S^i$  and  $S^\alpha$  are formulated below. The slip system deformation resistances are taken to evolve in the form (Kalidindi et al., 1992):

$$S^i(\tau) = S^i(t) + \sum_j h_{sl}^{ij}(t) \Delta\gamma_{sl}^j, \quad \text{where } h_{sl}^{ij} = q_{sl}^{ij} h_{sl}^j. \quad (12)$$

here  $h_{sl}^{ij}$  are components of the hardening matrix,

$$q_{sl}^{ij} = [q_{sl} + (1 - q_{sl}) \delta^{ij}] \quad (13)$$

is the matrix describing the latent hardening, with  $q_{sl} = 1.0$  for co-planar systems and  $q_{sl} = 1.4$  for non-coplanar systems, and

$$h_{sl}^j = h_{sl,0} \left( 1 - \frac{S_{sl}^j}{S_{sl}} \right)^{a_{sl}} \quad (14)$$

is the single slip hardening rate. So we have  $\{h_{sl,0}, S_{sl}, a_{sl}\}$  as hardening parameters for dislocation slip, which are taken to be identical for all slip systems. The twin system deformation resistances are taken to evolve in the form

$$S^\alpha(\tau) = S^\alpha(t) + \sum_j h_{tw}^{\alpha j}(t) \Delta\gamma_{tw}^j, \quad \text{where } h_{tw}^{\alpha j} = q_{tw}^{\alpha j} h_{tw}^j. \quad (15)$$

Similarly,  $h_{tw}^{ij}$  are the components of the hardening matrix by deformation twinning, and

$$q_{tw}^{\alpha j} = [q_{tw} + (1 - q_{tw}) \delta^{\alpha j}] \quad (16)$$

is the latent hardening matrix, with  $q_{tw} = 1.0$  for co-planar systems and  $q_{tw} = 1.4$  for non-coplanar systems. For the single twinning hardening rate,

$$h_{tw}^j = h_{tw,0} \left( 1 - \frac{S_{tw}^j}{S_{tw}} \right)^{a_{tw}}. \quad (17)$$

The three  $\{h_{tw,0}, S_{tw}, a_{tw}\}$  hardening parameters are taken to be identical for all twinning systems.

Twinning is considered as pseudo-slip. Different to dislocation slip, however, deformation twinning will result in the rotation of the lattice in the region of the crystal that has gone through twinning (Kelly and Knowles, 2012; Pitteri, 1985, 1986). For TWIP steels, we consider the twin elements  $\{\mathbf{K}_1, \mathbf{K}_2, \boldsymbol{\eta}_1, \boldsymbol{\eta}_2\}$  defined by

$$\mathbf{K}_1 = (111), \quad \boldsymbol{\eta}_1 = [11\bar{2}], \quad \mathbf{K}_2 = (11\bar{1}), \quad \boldsymbol{\eta}_2 = [112]. \quad (18)$$

With the definition of  $\mathbf{p}$  being a unit vector in the  $\boldsymbol{\eta}_1 = [11\bar{2}]$  direction, and  $\mathbf{q}$  being the unit normal to the  $\mathbf{K}_1 = (111)$  plane. The rotations which carry the matrix lattice to twinned lattice and the inverse (or detwinning) are respectively given by,

$$\mathbf{R}^{tw} = 2\mathbf{q} \otimes \mathbf{q} - 1 \quad \text{and} \quad \mathbf{R}^{dw} = 2\mathbf{p} \otimes \mathbf{p} - 1. \quad (19)$$

That is, if  $\mathbf{x}_a$  are the lattice vectors of the matrix crystal, then the lattice vectors in the twinned region are given by  $\mathbf{e}_a = \mathbf{R}^{tw} \mathbf{x}_a$ . As soon as the accumulative pseudo-slip in a twinning system reaches the threshold strain  $0.5e^T$ , we will rotate the matrix lattice to the twinned lattice in each single crystal. Further details can be found in Staroselsky and Anand (1998), Staroselsky (1998).

## 5. Numerical modeling on deformation mechanisms in TWIP steels

Now we use the constitutive model summarized above to simulate the mechanical deformation of TWIP steels with large plasticity. Material parameters are abstracted by fitting the experiments results in RD. We then explore the roles by each mechanism at different stages of plastic deformation, and test the predictability of the model to deformation in ND. Given the large deformability of the materials and the grain sizes are in tens of micrometers, we neglect the influence of grain boundary deformation, as the latter usually results in premature failure and low ductility. That means that grains in our samples are rigidly bonded. Detailed material parameters include

- Elastic properties: the used values of elastic constants for FeMnC are  $C_{11} = 235.5$  GPa,  $C_{12} = 138.0$  GPa,  $C_{44} = 117.0$  GPa (Gebhardt et al., 2011; Idrissi et al., 2010a).
- Slip/twinning systems: the 12 slip systems in FCC crystals are  $\{111\}\langle 110\rangle$ , the 12 twin systems in FCC crystal are  $\{111\}\langle 11\bar{2}\rangle$ .

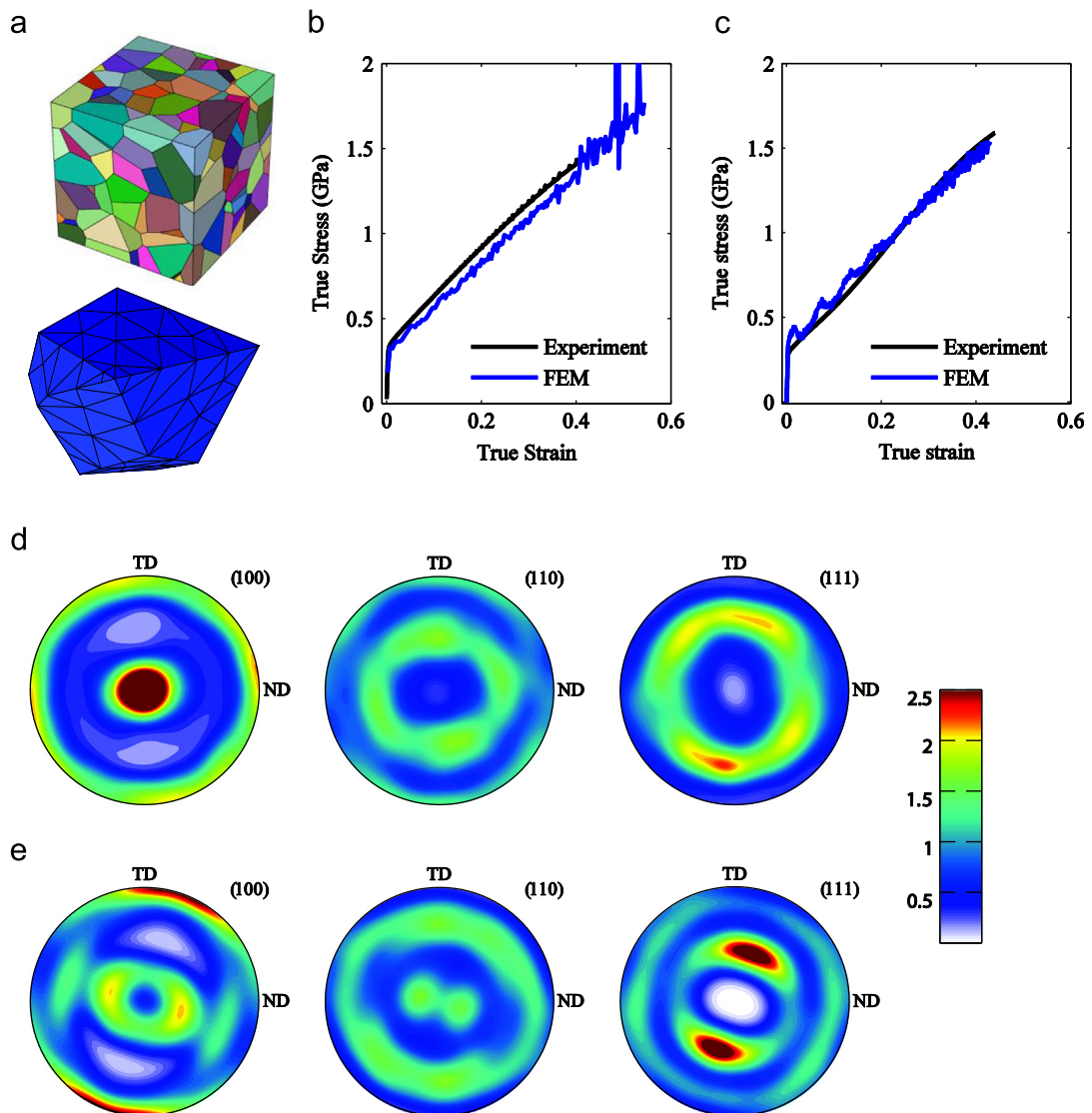


- Initial slip/twinning resistances: {121 MPa} for slip and {70 MPa} for twin. These numbers reflect the factor that the nucleation of leading partial dislocations for twins is much easier than the generation of complete dislocations. These numbers are calibrated to ensure experimentally measured stress–strain curves and texture at a given strain match well with simulated results when deformation is applied along the RD direction.
- Initial texture: the experimentally measured orientation data (Fig. 5) for the as received FeMnC are discretized into 300 orientations for the 300 Voronoi grains.
- Hardening parameters for slip and twinning: in the power-law hardening, we have three parameters  $\{h_{sl,0}, S_{sl}, a_{sl}\}$  for slip induced hardening, and three parameters  $\{h_{tw,0}, S_{tw}, a_{tw}\}$  for twin induced hardening. Motivated by the mechanistic

**Table 3**

Two sets of strain hardening parameters used in the crystal plasticity model for our finite-element simulation.

	$S_0^i$ (MPa)	$h_{sl,0}$ (MPa)	$S_{sl}$ (GPa)	$a_{sl}$	$S_0^{tr}$ (MPa)	$h_{tw,0}$ (MPa)	$S_{tw}$ (GPa)	$a_{tw}$
Twin only	–	–	–	–	90	280	1	1.0
Twin & slip	121	400	2	0.25	70	2000	1.2	1.0



**Fig. 6.** Experimental results versus simulated results for FeMnC TWIP steel while straining in RD direction. Here we only consider plasticity by deformation twinning. (a) Initial microstructures and typical mesh in a grain. Stress–strain curves for (b) tension and (c) for compression. Crystallographic texture for FeMnC from simulations. (d) Texture after 56% tensile strain. (e) Texture after 43% compressive strain.

model for strain hardening by deformation twinning (Eq. 7), we have used a linear hardening law for deformation twinning, i.e.  $a_{tw} = 1$  in Eq. (17).

To get a clear picture about the role played by each mechanism for hardening, we do not take the cross-hardening into account in the present study. The readers are referred to a more sophisticated treatment for cross-hardening in crystal plasticity models considering both twinning and dislocation slip (Fernández et al., 2011). We have used two sets of material parameters to capture the strain hardening in TWIP steel FeMnC: in one case, we suppress dislocation induced plasticity and see whether deformation twinning alone can capture the stress–strain behavior and the texture evolution of the material. Both dislocation slip and deformation twinning are activated in the second case. Corresponding hardening parameters for both cases are listed in Table 3.

In Fig. 6a, we show the polycrystalline microstructure used for all simulations. The mesh of a typical grain is also given at the bottom in Fig. 6a. We first explore the stress–strain behavior by taking into account plasticity by deformation twinning alone. A reasonable match between the stress–strain curves from experiments and those from modeling is observed. Fig. 6b

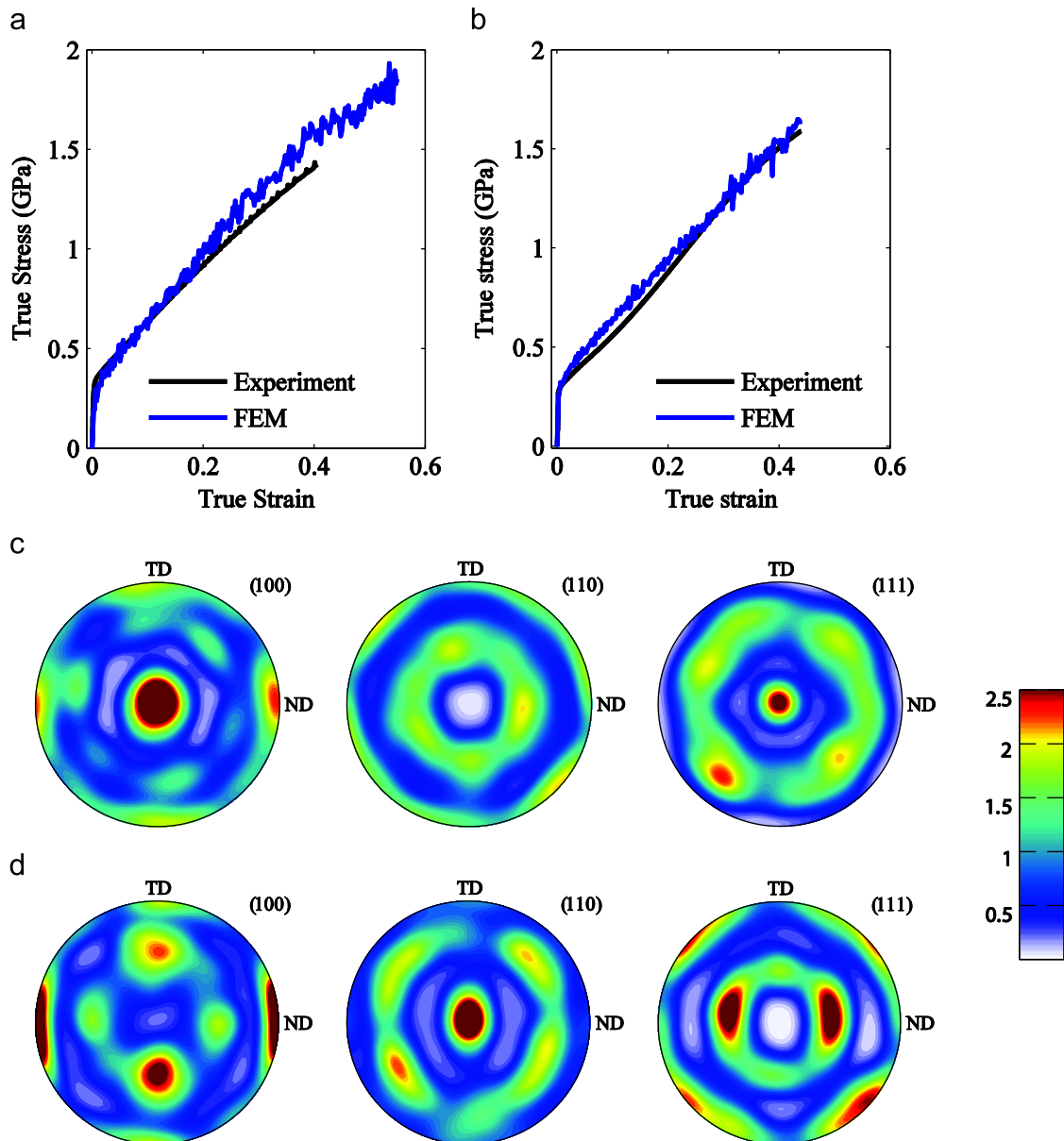
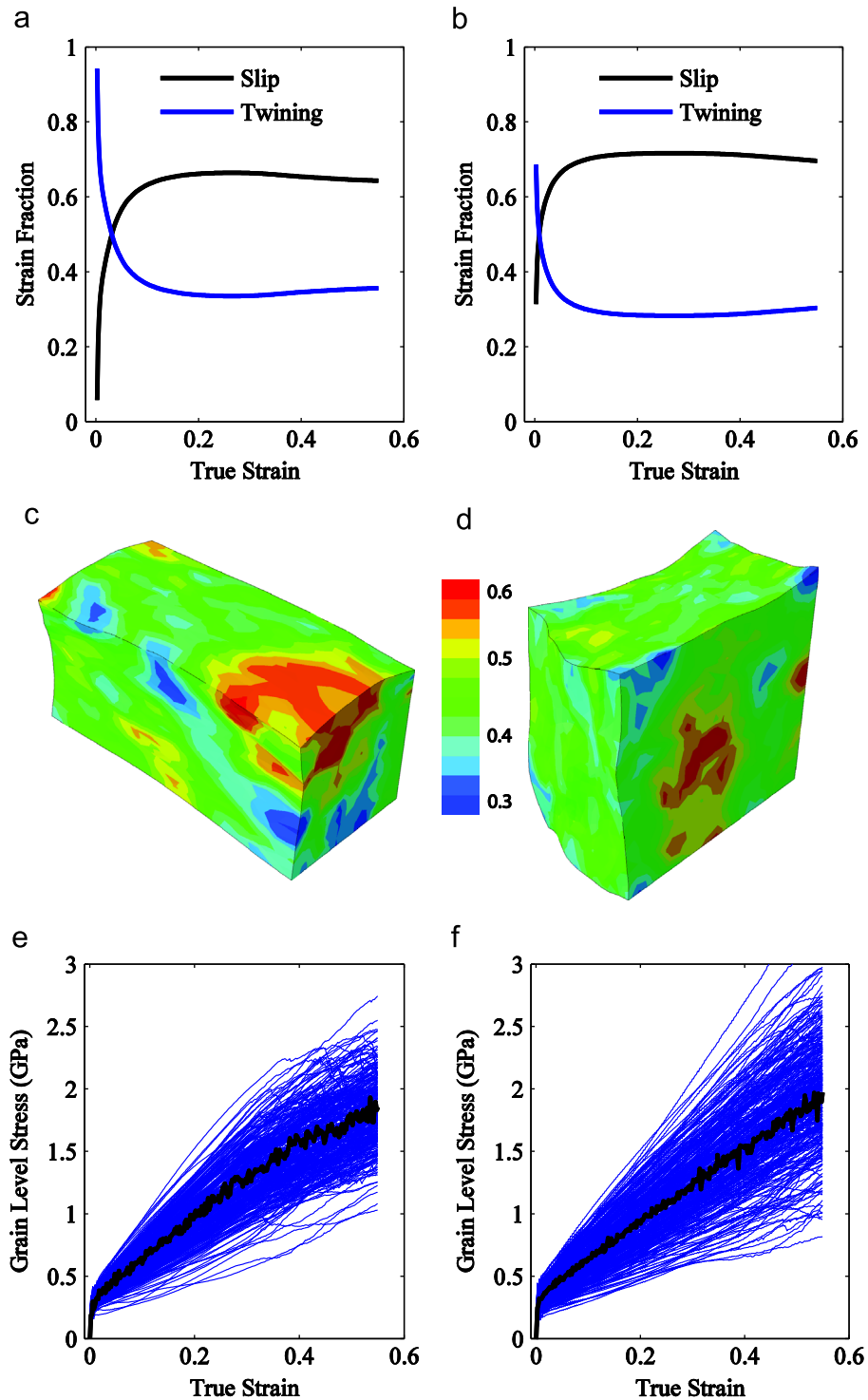


Fig. 7. Experiments versus simulated results by considering both dislocation slip and deformation twinning in RD direction. Stress–strain behavior: (a) tensile stress–strain curves, and (b) compressive stress–strain curves. Texture evolution: (c) texture at 56% tensile strain, simulation, and (d) texture at 43% compressive strain, simulation.

presents the stress–strain curves in tension, and the compressive stress–strain curves are given in Fig. 6c. As plastic deformation increases, the 12 twin resistances increase correspondingly from 90 MPa to about  $548 \pm 96$  MPa at a true strain of 0.56 in tensile tests, and it increases to  $460 \pm 62$  MPa at a true strain of  $-0.43$  in compressive. By further checking the



**Fig. 8.** Detailed grain level deformation from simulations while loading along the RD direction. (a) The fractional plastic strain contributed by individual mechanisms during tension. (b) Evolution of fractional plastic strain during compression. Contours of equivalent plastic strain at (c) 56% tensile strain, and (d) at 43% compressive strain. Grain level stress as a function of strain during (e) tension and (f) compression. Blue lines are for average stresses along the loading axis for individual grains, and the black line is the macroscopic stress–strain response of the sample. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

crystallographic textures for FeMnC after deformation, the results from our simulations (Fig. 6d for tension and 6e for compression) differ from the experimental measurements in Fig. 5: The strong {111} texture fiber is missing. The inconsistency in texture evolution implies that deformation twinning may be not the single carrier for plasticity.

By activating both dislocation slip and deformation twinning in the constitutive model, we show in Fig. 7 the simulated stress–strain curves again experimental results, with Fig. 7a for tension and Fig. 7b for compression. A nice match in stress–strain curves between our simulations and the experimental results is obtained by using the material parameters given in Table 3. Interestingly, stress–strain curves from our simulations also capture the increasing strain hardening modulus with straining, which is regarded as a crucial factor for the large ductility in TWIP steels. The {100}, {110}, and {111} pole figures for quasi-static tension and for quasi-static compression are shown in Fig. 7c and d; the {100}, {110} and {111} pole figures are very much alike between the numerical prediction and experimental measurements (Fig. 5b for tension and 5c for compression). To see the competition between the dislocation mechanism and the twinning deformation, we define two equivalent plastic strains, with

$$\Delta\bar{\gamma}_{sl} = \sqrt{(3/2)(\sum_i \Delta\gamma_{sl}^i S_0^i) : (\sum_i \Delta\gamma_{sl}^i S_0^i)}, \quad \Delta\gamma_{sl} = \int_0^\tau \Delta\bar{\gamma}_{sl} dt \tag{20a}$$

and

$$\Delta\bar{\gamma}_{tw} = \sqrt{(3/2)(\sum_\alpha \Delta\gamma_{tw}^\alpha S_0^\alpha) : (\sum_\alpha \Delta\gamma_{tw}^\alpha S_0^\alpha)}, \quad \Delta\gamma_{tw} = \int_0^\tau \Delta\bar{\gamma}_{tw} dt \tag{20b}$$

contributed by dislocation slip and deformation twinning, respectively. The evolution of fractional equivalent plastic strains as a function of the applied strain is shown in Fig. 8a for tension and 8b for compression. During the incipient of plastic deformation, we find that twinning dominates the plastic deformation and its fractional plastic strain reaches about 90% within 5% strain. The fractional strain by twinning drops quickly with straining while that by dislocation slip increases. Beyond 20% strain, both fractional strains reach their steady state: dislocation slip occupies about 65% of the overall plastic strain, and deformation twinning takes about 35%. That is to say, even the materials are named as ‘twinning induced plasticity steel’, more plastic deformation comes from dislocation slip, that circumstance only happens at the initial stage of plasticity. In Fig. 8c and d, we show the equivalent plastic strain contour at 56% tensile strain and 43% compressive strain, respectively. While there is no apparent shear localization at the grain level, severe inhomogeneity in plastic deformation is observed. The average stress at typical grains are shown in Fig. 8e (in tension) and 8f (in compression). Strong fluctuation for stress at the grain level is also seen, and the fluctuation becomes large at higher level stress.

So far, our simulations have shown the capability of the crystal plasticity model to capture the essence of deformation characteristics in TWIP steel with severe plastic deformation. Now we aim to testify its predictability. We consider the same material but investigate its deformation in the ND direction. To be consistent, we use the same material parameters for previous simulations for the deformation in the RD direction. The initial texture for the sample in ND, together with those after 29% compressive strain, are shown in Fig. 9a and 9b, respectively. Due to the limitation of sample size, we are not able to measure the texture of samples after tension.

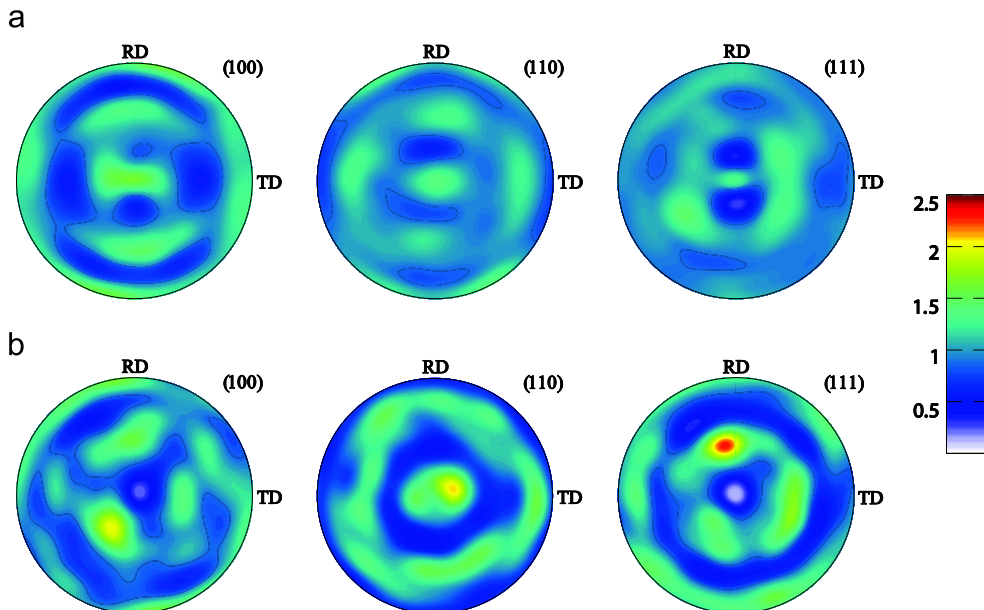


Fig. 9. Evolution of crystallographic texture for FeMnC from experiments while loading along the ND direction. (a) Initial texture. (b) Texture at 29% compressive strain, experiment.

Fig. 10 shows the stress–strain curves from FEM simulation when both dislocation slip and deformation twinning are activated, with Fig. 10a for tension and 10b for compression. Numerical predictions agree well with experimental results for the stress–strain responses in the ND direction. The texture evolutions from FEM simulations are shown in Fig. 10c and d, corresponding to texture at 52% tensile strain and 29% compressive strain, respectively. Texture at 29% compressive strain from our simulation also matches well with our experimental measurement shown in Fig. 9b. In particular, the primary (110) texture is captured nicely with the 300 initial orientations we used. We expect that even better match in stress–strain behavior and texture evolution can be achieved if systems with more representative grains can be simulated.

In Fig. 11a and b, we show the corresponding accumulative fractional strains as a function of the applied strain for tension and for compression in the ND direction, respectively. Similar to our observation when deformation is applied along the RD direction, deformation twinning has a smaller contribution to the overall plastic deformation when the macroscopic strain applied along the ND is greater than 20%. Corresponding equivalent plastic strain contour at 52% tensile strain and 29% compressive strain are shown, respectively, in Fig. 11c and d. While there exists a certain level inhomogeneous deformation, we do not see shear localization. Accompanying with the deformation inhomogeneity, we also observe strong stress fluctuation in individual grains, as seen from the average stress in typical grains shown in Fig. 8e (for tension) and 8f (for compression).

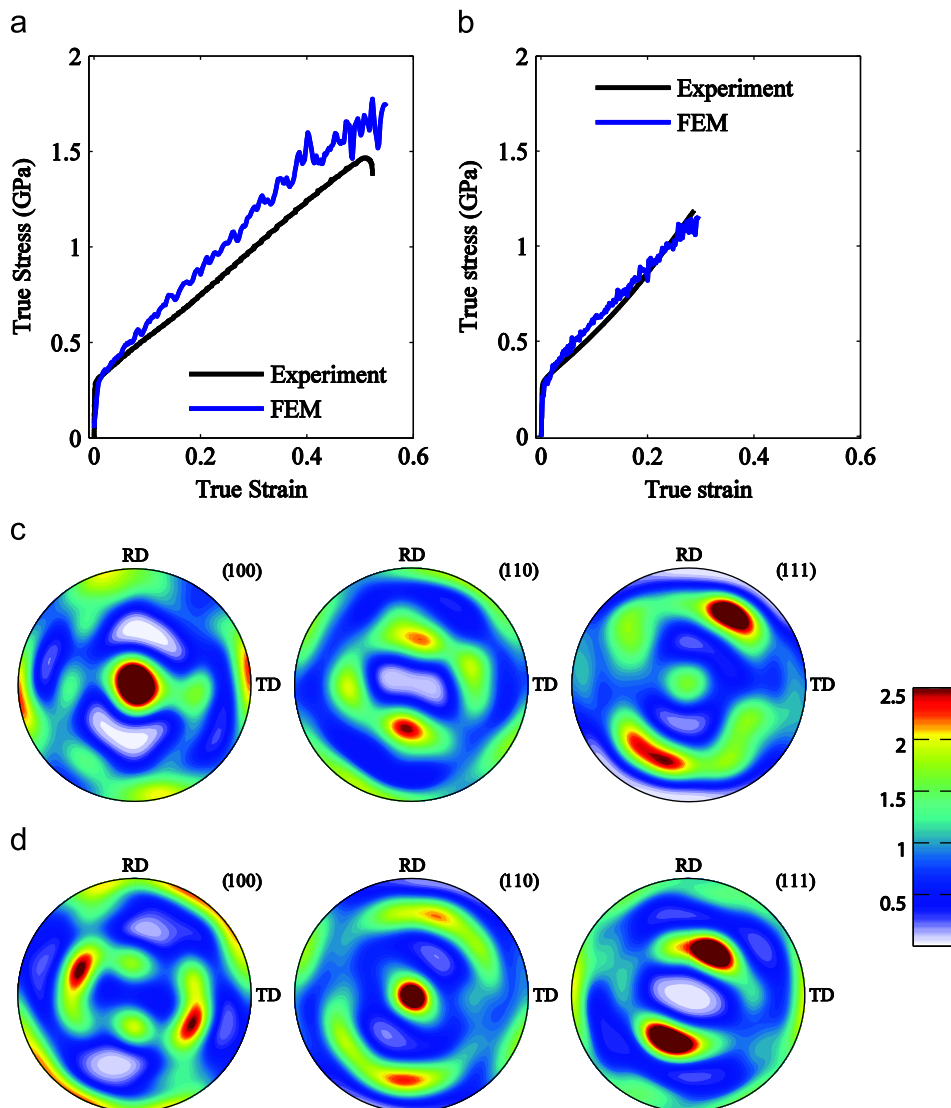
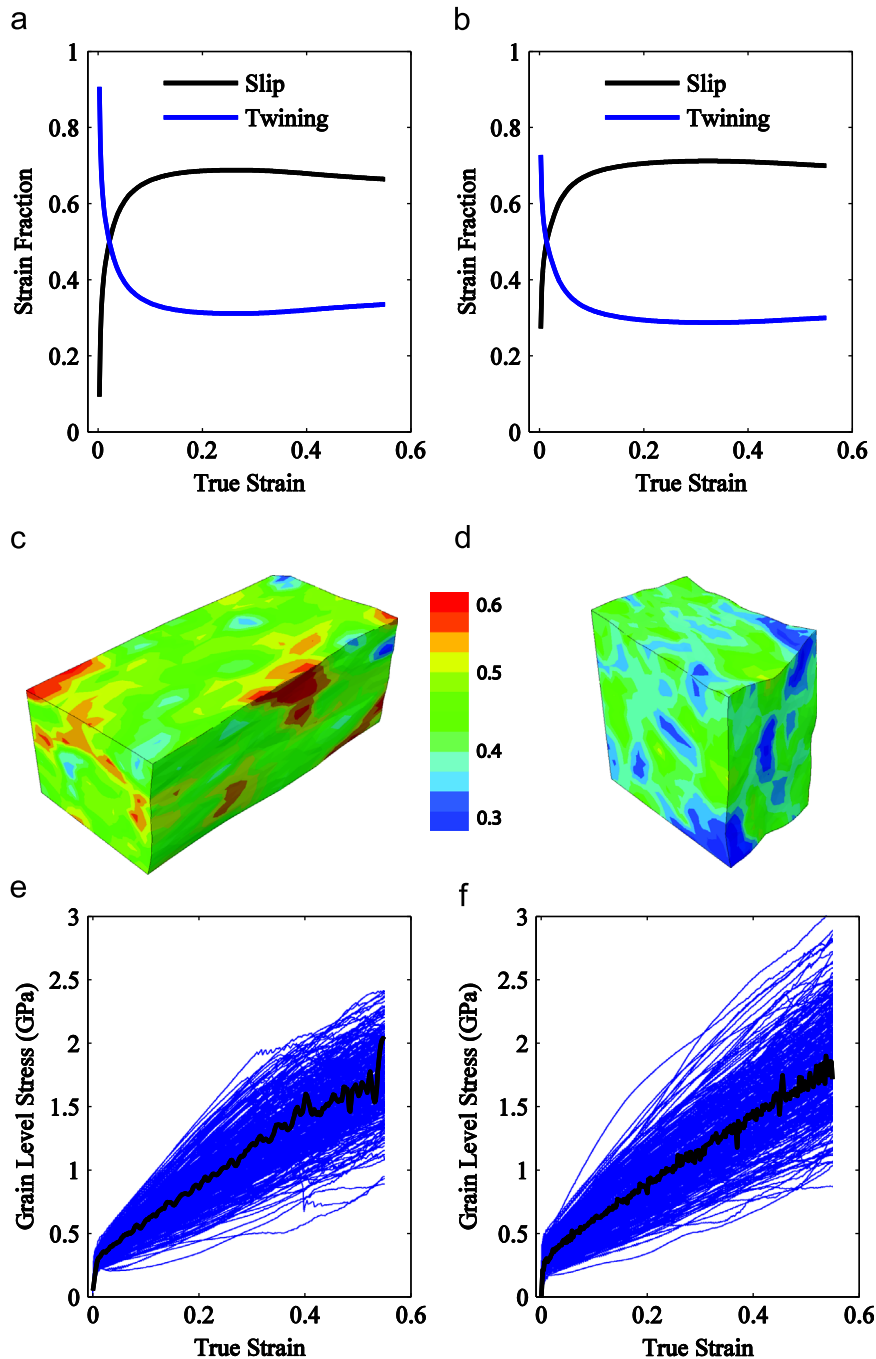


Fig. 10. Stress–strain curves and crystallographic texture for FeMnC when we apply loading along the ND direction. Both deformation twinning and dislocation slip are activated for plasticity. Stress–strain curves for (a) tension and (b) compression. (c) Texture at 52% tensile strain. (d) Texture at 29% compressive strain.



**Fig. 11.** Detailed grain level deformation from simulations while loading along the ND direction. (a) The fractional plastic strain contributed by individual mechanisms during tension. (b) Evolution of fractional plastic strain evolution during compression. Contours of equivalent plastic strain at (c) 52% tensile strain, and (d) at 29% compressive strain. Grain level stress as a function of strain during (e) tension and (f) compression. Blue lines are for average stresses along the loading axis for individual grains, and the black line is the macroscopic stress–strain response of the sample. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

## 6. Discussion and conclusion

In summary, we perform a systematic investigation on the strain hardening and texture evolution in high manganese TWIP steels, and develop a mechanistic model to explain the strain-hardening in crystals where deformation twinning dominates the plastic deformation. Using FeMnC TWIP steel, we show via both experimental measurements and finite-element simulations based on the classic crystal plasticity constitutive model, that deformation twinning plays a significant role for the strain hardening and texture evolution in TWIP steels. By including both deformation twinning and dislocation

slip, we obtain a good match between experimental measures and FEM simulations, for both stress–strain responses and texture evolution in TWIP steel during quasi-static deformation. While exploring the evolution of fractional strain with applied deformation, we find that twinning dominates the plastic deformation during the incipient of plasticity, and its fractional plastic strain reaches about 90% within 5% strain. The fractional strain by twinning drops quickly with straining while that by dislocation slip increases. Beyond 20% strain, both fractional strains seem to reach their steady state: dislocation slip occupies about 65% of the overall plastic strain, and deformation twinning takes about 35%. It indicates that even the materials are named as ‘twinning induced plasticity steel’; more plastic deformation comes from dislocation slip over that contributed by twinning during the late stage of plasticity. This observation is consistent with analysis that concurrent activation of alternative yet competitive deformation mechanisms like dislocation slip and twinning in some FCC metals is probable (Barbier et al., 2012, 2009a, 2009b; Chin et al., 1969; Gutierrez-Urrutia et al., 2010; Meng et al., 2007; Wei, 2011b; Yang et al., 2006). We further testify the predictability of the FEM calculations by considering the mechanical response and texture evolution of the TWIP steel along the ND direction. The numerical modeling shows good predictability when both dislocation slip and deformation twinning are involved in plastic deformation.

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