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Misorientation-Dependent Twinning Induced Hardening and Texture Evolution of TWIP Steel Sheet in Plastic Deformation Process

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Abstract: The quantitative contribution of twinning to hardening behavior and its effect on crystal orientation need to be explored in greater depth for design and forming of twinning-induced-plasticity (TWIP) steel products. To address this issue, the characteristics of twinning formation in the plastic deformation of Fe-30Mn-3Si-2Al TWIP steel are investigated in terms of intergranular misorientation distribution using electron back-scattering diffraction (EBSD), which reveals that most deformation twins adhere to the high-angle grain boundaries (HAGBs) of the face-center-cube (FCC) type TWIP steel. Texture measurements are conducted to show a stable volume fraction of major components including Goss, S and A orientations, while Copper shifts towards Brass orientation. A crystal plasticity finite element (CPFE) model based on virtual polycrystalline microstructure adopting representative volume element (RVE) is employed to simulate the deformation to reveal the correlation between misorientation-dependent twinning and hardening behavior of TWIP steel. The results demonstrate that the proportion of twinning hardening to overall hardening is larger than slip hardening. The stability of texture evolution is simulated to predict the anisotropy of TWIP steel. TWIP steel and thus is essential for accurate prediction of the mechanical behaviors.

Keywords: TWIP steel; crystal plasticity; twinning; misorientation; texture

1. Introduction

In automotive industries, development of new steels with desirable strength, ductility and toughness has been a hot research topic. Recently, low stacking fault energy (SFE) austenitic high Mn steels, which is regarded as a very attractive alloying element, has attracted a great deal of attention driven by the weight reduction and energy and materials saving in this industrial cluster [1–5]. Particularly, the application of a new generation of high Mn steels with Al and Si additions, called twinning induced plasticity (TWIP) steel, has been confirmed to efficiently realize weight reduction and energy saving due to their good mechanical properties to facilitate the down size of part dimension and size [3,6,7]. Greatly influenced by the content of chemical composition including Mn, Al and Si, various deformation mechanisms called TWIP and phase transformation induced plasticity (TRIP) effect related to the evolution of microstructure and crystallographic texture components should be considered as an important issue to be explored and addressed in the deformation process [3,8].

In terms of low-to-moderate SFE, Grässel et al. [9] observed that the extensive deformation twins play a dominant role for the austenitic high Mn steels alloyed with Si and Al. It is proposed that the TWIP effect significantly influences the hardening behavior at macroscopic level through

the interaction of dislocations gliding hindered by twinning boundaries when the Mn content is more than 25 wt %; the Al content is about 3 wt %; the Si content is between 2 wt % and 3 wt %; and the C content is low [9]. The impressive strain-hardening of TWIP steels is caused by various strengthening mechanisms, mainly consisting of dislocations glide and twinning [9], dynamic strain ageing [10] and TRIP-effect [11]. Among these mechanisms, twinning has been seriously taken into account and quantified to explain the strain hardening of TWIP steels, including the texture hardening [12], the dynamic Hall–Petch hardening [13] and the Basinski-type hardening [14]. However, there is still no consensus on the fundamental mechanisms of strain hardening in TWIP steels and the abovementioned studies strongly depend on the microstructural characteristics of twinning, but this issue is still under debate. Thus, it is essential to determine the location and distribution of twinning first. On the other hand, the deformation twins, which are regarded as an important lattice defect of TWIP steels, strongly affects the microscopic evolution especially for the crystallographic texture development in plastic deformation [15]. From the perspective of deformation mechanism, a remarkable characteristic associated with the deformation twins is the sudden reorientation of crystallites, leading to the preferred crystallographic orientation or texture component. Subsequently, the evolution of crystallographic texture contributes to strengthening generally via slip activities, known as texture hardening, to enhance the mechanical properties such as high strength and good ductility [16]. Through the thickness addition of nano-twins, the accumulation of the twin volume fraction could make contribution to crystallographic texture evolution [10], but how the deformation twins affect the strain hardening via the texture development in the course of deformation has not yet been extensively explored. Consequently, it is necessary to investigate the texture components and deformation twins' nucleation position first in the large plastic deformation process to establish a close connection among deformation twins, crystallographic texture components and strain hardening. However, this relationship has not been explored in greater depth and needs an in-depth investigation to correlate the microstructural characteristics of twinning and textural evolution with strain hardening, particularly for the Fe-Mn-Si-Al TWIP steels.

Since the anisotropy associated crystallographic texture is important in plastic deformation processing [5,17], it is indispensable to know more about the relation between crystallographic texture evolution and the microstructure formation and evolution. Currently, most studies on TWIP steels are focused on this relationship of Fe-Mn-C and Fe-Mn-Si-Al steels [18,19] and the investigations are more on the effect of crystallographic texture on deformation twins. Earlier experimental investigations detailing the uniaxial tensile loading of fine-grained Fe-Mn-C TWIP steel have revealed that the development of the pronounced <111> fiber in the tensile direction facilitates the formation of deformation twins and maintains the strain hardening rate at a high level [20]. However, the influence of twinning on texture development needs to be paid more attentions. For the Fe-Mn-Al-C TWIP steels, Souza et al. suggested that the texture transition from copper to brass texture was observed at higher reduction influenced by deformation twins with strong similarity to that found in Fe-Mn-C TWIP steels [21]. However, this issue should be investigated for Fe-Mn-Si-Al TWIP steels. Compared with Fe-Mn-C TWIP steels, the texture of Fe-Mn-Si-Al TWIP steels shows a great difference in tensile deformation process due to the lower magnitude of the activated twin systems [22]. Furthermore, Saleh et al. proposed that the texture measurement of Fe-Mn-Si-Al TWIP steels subjected to the uniaxial tension demonstrated the characteristic double fiber texture for FCC materials, with a relatively stronger <111> and a weaker <100> partial fiber parallel to the tensile axis [23]. However, a detailed explanation of texture transition affected by twinning has not been studied in these studies.

Based on the long-range interactions of individual grains with the polycrystalline aggregate [24], another widely used approach for predicting crystallographic texture is the viscoplastic self-consistent (VPSC) plasticity model. Through applying predominant twin reorientation (PTR) schemes [25] and CP (crystal plasticity) model proposed by Kalidindi [26] to deal with the twinning evolution, a VPSC model was presented by Prakash et al. [27] to investigate the influence of deformation twins on the crystallographic texture development after tensile loading. However, compared with Kalidindi

model, a limited correspondence between the experimental texture intensity and the simulated one obtained by the simulation using VPSC model and considering PTR scheme was concluded. Consequently, Saleh et al. [23] applied a modified VPSC model to assess the contributions of perfect and/or partial slip, twinning and latent hardening to evolution of the crystallographic texture in TWIP steels and overcame the limited correspondence between experiment and simulation via proper description of hardening parameters of various deformation systems. However, this "mean-field" approach for VPSC model has limitation as there is no sufficient information about the specific interaction between the individual grain and its neighboring grains [28,29]. Considering this limitation, a non-homogenization scheme based CPFE method was proposed to represent the intragranular microstructure and grain orientations. Furthermore, this approach facilitates taking into account the grain morphology of metallic materials in microstructural simulation [30,31]. To model the relationship between crystallographic texture and deformation twins' evolution, Dancette et al. [32] employed a "full-field" and experimental dataset based CPFE analysis to provide an improved prediction of the texture development in uniaxial tension at macroscopic scale, and the relation between the volume fraction of twins inside the individual grains and crystallographic texture at the grain level were confirmed via EBSD measurement and CPFE simulation. The introduced crystal plasticity (CP) model proved that it gives an improved texture prediction compared to the Taylor model for the deformation at higher strain.

In the present study, the grain morphology, crystal orientation and crystallographic texture evolution of Fe-30Mn-3Si-2Al TWIP steel under the uniaxial tensile deformation was studied via EBSD measurement, especially for the deformation twins' nucleation position and intra- and intergranular deformation. The corresponding CPFE model considering slip and twinning interactions was then proposed. Subsequently, the simulations using Voronoi based polycrystalline RVE microstructure with crystal orientations were conducted to investigate the evolution of hardening behavior associated with slip and twinning activity and further to discuss the effect of twinning on hardening and crystal orientation, as well as the stability of the crystallographic texture development. This study links the mechanical behaviors with microstructural change and texture evolution during deformation thereby provides an accurate prediction of the shape of forming parts in deformation processing of TWIP steels.

2. Experiments and Characterization

2.1. Material and Experimental Procedure

The kind of Fe-Mn-Si-Al TWIP steel was selected as the case study material. A vacuum induction furnace was used to manufacture the investigated steel with the chemical composition as listed in Table 1, detected by the spectral analysis. The tensile specimens with the gauge length of 20 mm, the gauge width of 10 mm, and the thickness of 0.5 mm were prepared by electron discharge machining of the fabricated steel sheets. The samples were then suitably annealed at the temperature of 800 °C for a fixed duration of 1 h and then followed by air cooling.

 Table 1. Chemical composition (in weight percent) of the Fe-30Mn-3Si-2Al TWIP (twinning-induced-plasticity) steel sample.

С	Mn	Si	Al	S	Р	Ti	Fe
0.11	30.5	2.88	2.34	0.013	0.007	≤ 0.01	Bal.

The tensile tests were conducted on a mechanical testing system with the pre-set constant crosshead speed of 6.9×10^{-3} mm/s in the tensile direction parallel to the rolling direction (RD). The tests were done with the engineering strain of 0.05, 0.1, 0.2 and 0.4. During the deformation process, a contactless laser extensometer was used to calibrate and measure the deformation strain of the testing samples.

Grain morphology and crystal orientation were characterized before deformation by using optical microscopy (OM, Olympus, Beijing, China) and EBSD techniques, respectively. The specimens were mechanically polished using the standard method along the longitudinal section (the plane normal to transverse direction) and etched in an alcoholic solution consisting of 5% nitric acid. OM morphologies demonstrated the equiaxed austenite grains with the average grain size of 30 µm (excluding twins) for the homogenized sample shown in Figure 1. The samples were electrochemically polished in 5% perchloric acid alcoholic solution for EBSD preparation. The EBSD scans were run over an area of 190 µm by 170 µm with the step size of 1 µm using a field emission Zeiss Auriga scanning electron microscope (SEM, Zeiss, Oberkochen, Baden-Württemberg, Germany) with a HKL camera. The total number of grains is about 100. The working distance was set to be 16 mm. The number of data points considered for the calculation of the ODFs is about 38,711. Grain boundaries from both the un-deformed and deformed specimens were identified with misorientation greater than 5° by a cleaning procedure consisting of grain confidence index standardization, whereas the standard Brandon's criterion [33,34] was used to identify the coincident site lattice boundaries. Furthermore, the high-angle grain boundaries (HAGBs) in EBSD orientation maps were defined to have the misorientation larger than 15° and the low-angle grain boundaries (LAGBs) have the misorientation between 2° and 15°. The EBSD data were used for calculation of the pole figures (PFs), inverse pole figures (IPFs), orientation distribution functions (ODFs), and texture components. The grain size was measured according to the criteria of grain reconstruction provided by the HKL Channel 5 software (Oxford Instrument, Witney, Oxon, UK). These results were applied to understand the crystal orientations evolution and the crystallographic texture development in deformation process.

2.2. Results

2.2.1. Misorientation-Dependent Twinning Characteristics

Figure 1 shows the OM of the as-annealed TWIP steel and a large number of annealing twin lamellae could be clearly distinguished in the microstructure. Statistical analyses show Fe-30Mn-3Si-2Al-0.11C steel has an average grain size of ~30 μ m. The subsequently EBSD observations were conducted on RD × TD plane of the initial-state sample, providing crystal orientations, grain size distribution, and confirmed that the sample has fine-grained structure as shown in Figure 2a,b. The morphologies of the annealing twins are lath-shaped characteristically (Figure 2a), while the deformation twins often appear in lenticular and its boundaries in clusters. The experimental (111), (110) and (100) PF plots in Figure 2c indicated that the initial crystallographic orientations of annealed specimen are approximately stochastic distributed scatters, which represents that weak textures exist in the annealed samples.



Figure 1. Morphology of the Fe-30Mn-3Si-2Al-0.11C steel annealed at the temperature 800 °C for 1 h.



Figure 2. (a) EBSD (electron back-scattering diffraction) imaging map cropping from RD × TD plane; (b) Statistics of grain size distribution; and (c) Experimental (111), (110) and (100) PFs (pole figures) of the annealed TWIP(twinning-induced-plasticity) steel samples.

To efficiently determine the position of twin lamellae, it is established that twin lamellae is often originated from a statistical distribution of defects in the grain boundaries [35,36]. Particularly the grain boundary misorientation angle exhibits a significant influence on the probability of twin nucleation. Thus, the locations of twin lamellae could be determined approximately via recording the distributions of the intergranular misorientations angle. For the EBSD analysis, as illustrated in Figure 3c, the misorientation angles between the adjacent grains of specimen with the tension strain of 0.1 are above 15°, and mostly above 60°, which illustrates the majority of grain boundaries belonging to HAGBs, including the twinning grain boundaries (TGBs). A visualization of grain boundary misorientation of the sample with the strain of 0.1 is shown in Figure 4c. Indeed, the number of HAGBs represented by red color code is larger than that of LAGBs highlighted by blue color code. In addition, it is observed that, for the uniaxial tensile loading condition, mostly twin lamellae in the FCC-type phase were originated in the HAGBs above 25°.



Figure 3. Misorientation angles distribution within grains of the specimen with the tension strains of: 0.1 (**a**); and 0.4 (**b**). Misorientation angles distribution between adjacent grains with the tension strains of: 0.1 (**c**); and 0.4 (**d**).

With the increase of strain to 0.4, as shown in Figure 3d, the misorientation angles above 60° exhibit a decreasing tendency from 55% to 40%. It is noted that the deformation twins are attached to the HAGBs of the distorted grains, as labeled with arrows in Figure 4d. It could qualitatively conclude that twin lamellae mostly adhere to HAGBs for a FCC-type TWIP steel undergoing uniaxial tensile deformation. During the plastic deformation process, the deformation compatibility of neighboring grains could lead to the activation of accommodative slip systems, twinning and the reorientation of the parent grains. The lattice rotation in the near-boundary zones is impeded by neighboring grains, resulting in the formation of lattice curvatures between the near-boundary zones and the center zones of grains [37]. Thus, the substructures such as the uneven distributions of twinning boundaries and twinning variants would cause heterogeneity within the individual grains. The intragranular misorientations thus evolved with the strain from 0.1 to 0.4, as shown in Figure 3a,b, respectively. It is noted that the major distributions of intragranular misorientation at the strain of 0.1 are located in low angles (below 15°) by comparing Figure 3a,b. With increasing tensile strain to 0.4, it is noted that a similar statistical distribution of the intragranular misorientation could be observed except for a slight difference in quantity. The change in the intragranular misorientation corresponds to the stored energy of cold deformation and the formation of LAGBs. The detailed discuss is given. The intragranular misorientation reflects strain generated during deformation with dislocation glide, particularly related to the density of geometrically necessary dislocations [38,39]. With the increasing strain from 0.1 to 0.4, the dislocation accumulation would occur at the grain boundaries via dislocation gliding, which generates local stress and leads to inhomogeneous deformation at the grain boundaries. The LAGBs are thus supposed to emerge.

In addition, the strain-induced intragranular misorientation is strongly related to the grain orientation which changes constantly with the increasing strain [40]. It is also well-known that the stored energy depends on crystallographic orientation and plays a significant rule in the formation of texture [39]. Thus, the intragranular misorientation corresponds to the stored energy indirectly. Based on the above analysis, the change of intragranular misorientation is closely related to the formation of LAGBs and the stored energy.



Figure 4. Visualization of the intragranular misorientations with the strains of: 0.1 (**a**); and 0.4 (**b**). The distribution of grain boundary misorientations with the strains of: 0.1 (**c**); and 0.4 (**d**).

2.2.2. Crystallographic Texture Evolution

To get a complete description of the crystallographic texture evolution, ODFs were calculated based on the experimental PFs using the series expansion method [41]. For the cold-rolled FCC-type metallic materials such as TWIP steel investigated in the present study, it is well-established that the main texture components generally consists of Cu-{112}<111>, S-type {123}<634>, Goss-{110}<001> and Brass-{110}<112> components. To present the gradual transition of texture of the polycrystalline FCC materials, the partially ideal and important texture components are labeled schematically for the sections of ODFs with $\phi_2 = 0^\circ$, 45° and 60° in Figure 5, as well as the corresponding experimental ODFs with the tensile strain from 0.05 to 0.4, as well as the initial state.



Figure 5. Texture development at the strain of 0.05, 0.1, 0.2, and 0.4; the shown sections of ODFs (orientation distribution functions) for $\phi_2 = 0^\circ$, 45° , 60° determined by EBSD; and the important texture components in FCC (face-center-cube) materials.

As seen in Figure 5 with the strain of 0.05, the starting deformation texture is comprised mainly of A ({110}<556>) orientation, Brass (B) orientation along α -fiber, as well as Copper (Cu) and S ({123}<634>) orientation. With the greater tensile strain of 0.1, a pronounced increase in the intensity of the A {110}<556> orientation was found in the α -fiber of $\phi_2 = 45^\circ$ ODF figures. Meanwhile, the B orientation also shows an apparent increase in the intensity with the increasing tensile strain. With the strain larger than 0.2, the main textures consist of Goss ({110}<001>) and B orientations. This observation is consistent with the texture evolutions in the conventional FCC materials after uniaxial tension [23]. In addition, a weakened {112}<111> component is also identified. With the increase of tensile strain to 0.4, the main texture components are similar to those observed in the specimen deformed to the strain of 0.2. However, the intensity of several orientations becomes stronger. At this level, an important feature is the remarkable enhancement of the intensity for {112}<111> copper orientation. In addition, another feature is the further decreasing {110}<556> A orientation.

To quantify the stability of the main textures in tensile deformation, the volume fraction of each texture component is plotted as a function of tensile strain, as shown in Figure 6. Indeed, the Cu and A components show a large majority comparing with G and B textures. It is noted that the volume fraction of A and G orientations were found to remain nearly stable during the uniaxial tension although there is a slight decrease with the strain of 0.1. However, the Cu orientation exhibits a large decrease in volume fraction while a smaller increase in volume fraction is illustrated for B orientation. Actually, the evolution of such a texture is mainly attributed to the occurrence of deformation twinning,

despite of the fact that slip also contributes to the development of B orientation [42,43]. The Cu orientation could twin to form the Cu twin orientation (552)<115>, which is transformed to the Goss orientation, and, finally, to the B orientation [44,45]. Based on thisanalysis, as for TWIP steels, Bracke et al. [43] have proposed that the Cu twin is the result of the twinning of Cu orientation, and it is not resulted from any other deformation mechanism. Therefore, the presence of the B orientation in TWIP steel can be attributed to twinning. Moreover, it was proposed that twinning leads to planar slip and contributes to formation of B orientation [46].



Figure 6. The calculated volume fractions of the important texture components in the tension deformation of TWIP steels.

3. Microstructure-Based CPFE Modeling

3.1. Crystal Plasticity Model Including Slip and Twinning

It is well established that dislocations slip is considered as the main physical mechanism of crystal plastic deformation at room temperature, as well as deformation twinning. Developed based on dislocations and twinning evolution in crystals, the crystal plasticity (CP) constitutive model is widely adopted to represent the macro- and microscopic evolution of polycrystalline materials, particularly for representing the crystallographic texture development.

The basic framework including kinematics and dynamics adopted in the CP model follows the work of Kalidindi et al. [47]. In this paper, the plastic flow rule is established using rate-dependent approach. In the rate-dependent CP model, the shear rate of slip systems can be obtained directly by the decomposition of shear stress [48]:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left| \frac{\tau^{\alpha}}{s^{\alpha}} \right|^{1/m} \operatorname{sign}(\tau^{\alpha}) \tag{1}$$

where τ^{α} denotes the resolved shear stress (RSS) on the slip system α . s^{α} is the slip resistance for the slip system α . *m* is the strain rate sensitivity factor. $\dot{\gamma}_0$ is a reference slip shear rate, which is considered to be the same for all the slip systems [49].

The similar power law is adopted to describe the evolution of the shear rate of twinning systems:

$$\dot{\gamma}^{\beta} = \dot{\gamma}_{0}^{\beta} \left(\frac{\tau^{\beta}}{s_{\text{tw}}^{\beta}} \right)^{1/n}, \text{ if } \tau^{\beta} > 0; \quad \dot{\gamma}^{\beta} = 0, \text{ if } \tau^{\beta} \le 0$$
(2)

where s_{tw}^{β} and τ^{β} represent the twin resistance in a twin system and the RSS of that twin system, respectively. *n* is the strain rate sensitivity factor. $\dot{\gamma}_{0}^{\beta}$ is a reference shear rate of all the twinning systems.

The formulation of the hardening relation modeling of the evolution of FCC-type TWIP steel is presented. It is assumed the ratio between twin and slip resistance can be a constant which depends on the twin morphology based on the Hall–Petch explanation. Consequently, in this study, the twinning

resistance is considered proportionally to slip resistance. The evolution of slip resistance of the α th slip system is formulated as follows:

$$\dot{s}^{\alpha} = h_s^{\alpha} \left(1 - \frac{s^{\alpha}}{s_s^{\alpha}} \right) \sum_{\alpha=1}^{N_{\rm slip}} \dot{\gamma}^{\alpha}$$
(3)

where h_s^{α} and s_s^{α} represent the hardening rate and the saturated value associated with the slip system α , respectively. The extended hardening equations to capture the complex interactions of slip and twinning are given by [50]:

$$h_s^{\alpha} = h_s \left(1 + C \left(\sum f^{\beta} \right)^b \right) \tag{4}$$

$$s_s^{\alpha} = s_{s0} + s_{\rm pr} \left(\sum f^{\beta}\right)^{0.5} \tag{5}$$

where h_s indicates the initial hardening rate, *b* and *C* denote the hardening parameters of twinning system. s_{s0} represents the saturated value of slip resistance without twinning, s_{pr} indicates the parameter to reflect the effect of Hall–Petch mechanism, and f^{β} describes the twin volume fraction of the twinning system β .

The introduced CP constitutive model and integration algorithms are implemented numerically into the commercial finite element code ABAQUS standard via a user-defined material (UMAT) subroutine. A detailed Newton–Raphson iteration scheme could be seen in [7].

3.2. Establishment of Virtual Polycrystalline Microstructure

To represent the macro-scale response of specimen, a RVE model containing 100 grains, which are approximately consistent with the grain number in EBSD experiments, was employed to reconstruct the polycrystalline microstructure which considers the crystallographic orientation and morphological feature, as shown in Figure 7a. This virtual polycrystalline microstructure is generated using an open-source software package: Neper construct as the Voronoi tessellation model [51]. In Figure 7b, the FE model of this polycrystalline microstructure contains approximately 14,200 linear tetrahedral elements (C3D4 in ABAQUS, Dassault Systemes SIMULIA, Providence, RI, USA) since the use of higher-order elements does not have a significant influence on the stress-strain field and the prediction of crystallographic texture [52–54]. The polycrystalline model is then subjected to uniaxial tension up to the strain of 0.4. The initial un-deformed microstructure is illustrated in Figure 7b and the dimensions of the simulation model with 10 mm \times 10 mm \times 0.5 mm are given. As shown in Figure 7b, the simple tensile test was performed by imposing displacement in the X direction (the rolling direction, RD) with the lateral YZ plane fixed. Using trial and error tests, a set of the model material parameters are illustrated in Table 2, which summarizes the final values adopted for the material parameters of crystallographic slip and twinning together with elastic tensors. The methods for determining the elastic tensors (C_{11} , C_{12} , and C_{44}) of TWIP steel are referred to the studies by Pierce et al. [55] and Gebhardt et al. [56]. In addition, the plasticity parameters (h_s , S_{s0} , S_{pr} , b, C, S_0^{α} , S_0^{β}) are calibrated based on the stress-strain response. In the absence of enough experimental data to determine the plasticity parameters, a low strain rate sensitivity m = 0.02 and a reference strain rate $\dot{\gamma}_0 = 0.001 \text{ s}^{-1}$ are assumed [49]. The large hardening in the experimental response reveals a large initial hardening rate ($h_s = 180$ MPa) and a large saturation hardness ($S_{s0} = 300$ MPa). With the calibrated material parameters obtained by fitting the stress-strain curves performed with the strain of 0.4, the crystal orientations can be predicted to conduct the simulation.



Figure 7. Voronoi tessellation subjected to uniaxial tension. Colors represent different grains with different crystallographic orientations: (**a**) polycrystalline morphology; and (**b**) C3D4 mesh refinement with 100-grain polycrystals.

Initial hardening rate of slip system h_s (MPa)				
Saturated value of slip resistance without twinning S_{s0} (MPa)				
Hardening index of twinning b				
Hardening coefficient of twinning C	10			
Effect of Hall–Petch mechanism S_{pr} (MPa)	300			
Initial slip resistance S_0^{α} (MPa)	120			
Initial twinning resistance S_0^{β} (MPa)	139.2			
Elastic constant C_{11} (GPa)	198			
Elastic constant C_{12} (GPa)	125			
Elastic constant C_{44} (GPa)	122			
Rate sensitivity coefficient <i>m</i>	0.02			
Reference shear rate $\dot{\gamma}_0$ (s ⁻¹)	0.001			

Table 2. Material parameters in the constitutive relations calibrated for TWIP steel.

3.3. Evaluation of the CPFE Model

It is noted that the conventional way to calibrate the CPFE constitutive parameters in simulation is to establish a FE model which assumes that all elements consist of the same number of representative crystallographic orientations. However, the grain morphology such as intra- and intergranular misorientations could not well be reflected. Furthermore, the local deformation induced by individual grain properties also could not be reproduced. In this research, individual grains with orientations is generated and meshed in the FE model. Due to the limited computing power for simulations, modeling of a macroscopic specimen containing millions of grains and is then implemented within a FE model is difficult. Consequently, a RVE model containing grain morphology is proposed to represent the mechanical behavior of the macroscopic testing samples.

In this RVE model, each grain represents a specific crystallographic orientation and is composed of many elements. Instead of the conventional approach which directly assigning all the EBSD crystal orientations into RVE grain set, the crystal orientations used in this research were generated from discretizing ODFs using MTEX toolbox [57] in order to represent initial texture and to avoid the difficulty of selecting appropriate experimental orientations [58]. Subsequently, these orientations representing the texture were assigned to the RVE grains to describe an inhomogeneous material. Based on the microstructure and texture, the RVE model could capture the anisotropy characteristics of TWIP steel to bridge the gap between experiments and simulations.

To consolidate the simulated reliability, the comparison between the simulated and experimental intergranular misorientation and intragranular misorientation at the strain of 0.4 are shown in Figure 8. It is noted that a similar distribution of intergranular misorientation obtained by CPFE and EBSD could be observed. Meanwhile, the major boundary misorientation angles are above 15°, indicating there are a large number of HAGBs, as shown in Figure 8a. However, in Figure 8b, both the simulated and

experimental intragranular misorientation shows a high frequency of the low misorientation angle below 15°, which represents the approximate homogeneous orientation within the individual grain.



Figure 8. Comparison between simulated and experimental: (a) intergranular misorientation; and (b) intragranular misorientation at a strain of 0.4.

Based on the reliability of the established RVE model, as shown in Figure 9, it could be observed there is a good fitting to the experiments in terms of the stress–strain curve. Although there is a slight deviation with the true strain above 0.25, the hardening trend of the numerical simulation captures the main features of the experimental measurement. In this research, the modeling of initial grain orientations was simplified, but the experimental texture evolution indeed contributes to the hardening effect. In addition, although the serrated stress–strain curve has not yet appeared until the strain of 0.3, the dynamic strain aging might be taken place at larger strains probably. If so, the dynamic strain aging might make contributions to the overall hardening, which leads to a deviation between simulation and experiment. Finally, the coarse meshes and the calibrated parameters should be mentioned as the probable factors which could result in the deviation for the curves.



Figure 9. Comparison between simulation results by CPFE (crystal plasticity finite element) and experimental results from EBSD.

It is well established that twinning is considered as a significant role in the forming process of TWIP steels and its formation was dramatically influenced by the crystal orientations [20,22]. In addition, the evolution of microstructure (e.g., twinning) and texture components strongly relies on the crystal rotation. On the other hand, crystal orientations could be regarded as strong evidence to further verify the developed microstructure-dependent CPFE model. Then, a comparison of the simulated and measured PFs at different strains has been conducted in Figure 10. Figure 10 illustrates that the proposed CPFE model captures the main features of grain orientations of TWIP steels after the uniaxial tensile deformation to the strain of 0.4 well. It confirms that the macroscopic response and microscopic grain orientation distributions can be predicted and simulated by the microstructure-dependent CPFE model via introducing the initial experiment-based crystal orientations.





Figure 10. Comparisons of the (111), (110) and (100) PFs of TWIP steels obtained by the EBSD measurement (Experiment) and predicted by the microstructure-dependent CPFE model (Simulation) with the strain of 0.4.

4. Simulation and Discussion

4.1. Effect of Twinning on Hardening Evolution

The FE simulations of uniaxial tension were employed to validate the CP model for describing the twinning effect on hardening behavior and the evolution of slip and twinning in micro level, respectively. The equivalent von Mises stress distribution was calculated by the proposed CPFE model. It could be observed that there are non-uniform stress fields caused by various crystal orientations. In order to articulate the contributions of slip and twinning to the hardening evolution in each grain with experiment-based crystallographic orientation, the plot of the evolution of slip resistance is compared with the evolution of twin volume fraction to represent the individual hardening effect of slip and twinning to overall von Mises stress distribution in the simulated microstructure for the specimen deformed to the strain of 0.4, as shown in Figure 11.



Figure 11. (**a**) Von Mises stress distribution (stress concentration within the white dashed line region); (**b**) slip resistance; (**c**) twin volume fraction; and (**d**) twin resistance in the simulated microstructure of the sample stretched to the strain of 0.4.

The heterogeneous distribution of slip resistance exhibits a similar appearance compared with that of twin resistance, while the twin resistance shows a higher average intensity than slip resistance, shown in Figure 11b,d. It is noted that the similar distribution of von Mises stress and twin volume fraction was observed in simulation, as seen within the white dashed line region in Figure 11a,c. The proportion of twinned region to the overall RVE model is statistically 40% approximately according to the ratio of twinned grains to whole grains. Particularly, in Figure 11c, the grain with red color represents twin volume fraction shows a relatively higher value than other twinned regions, which shows the stress concentration. It indicated that the deformation twinning plays a significant role in the hardening effect of TWIP steel during uniaxial tensile process.

It is noted that, in Figure 12, the evolution of slip resistance and twin resistance represent an approximately parallel increasing trend, but the magnitude of twin resistance with initial value is larger than that of slip resistance. In Figure 12, the proportion of hardening due to twinning to overall hardening shows a decreasing trend with the increasing strain. Twins are considered as undeformable hard particles in austenitic matrix, acting as new obstacles for dislocation motions, leading to the so-called dynamic Hall–Petch effect. The obstacles including twinning boundaries impeded the dislocation slip so that the slip increment decreased and caused a reduced proportion of slip hardening to overall hardening.

Initiation of deformation twinning contributes to strain hardening through a dynamic Hall–Petch effect limiting the dislocation mean free path and consequently enhancing dislocation storage. However, with the increasing strain, when the twin volume fraction reaches the saturated value, this effect is not obvious. As shown in Figure 12, it is noted that a decreasing trend of the twinning hardening curve appears with the increasing strain, exactly revealing that the twin volume fraction gradually reaches the saturated value. Thus, the strengthening mechanism "dynamic Hall–Petch effect" caused by twinning provide limited contributions to overall hardening. However, to accommodate the further plastic deformation, the larger deformation resistance is needed, which leads to a higher strain hardening. On the other hand, based on the analysis of texture evolution, the presence of the Brass orientation in TWIP steel can be attributed to twinning. Generally, the twinned domain crystal lattice orientation, namely Brass orientation, is harder from the parent grain crystal orientation relative to the loading direction, which could be considered as the twinning induced texture hardening. Thus, the strain hardening of the studied TWIP steel is dominated by the combined influences of dynamic Hall–Petch effect at the initiation of deformation twinning and texture hardening when the twin volume fraction reaches the saturated value.



Figure 12. Evolution of the simulated slip and twin resistance at microscopic level and the proportion of slip hardening and twin hardening to overall hardening in the simulated microstructure of the sample with the strain of 0.4.

Based on the qualitative and quantitative analyses of the micro-deformation mechanisms and hardening behavior, for polycrystalline materials such as TWIP steels, the plastic deformation induced twinning leads to a decrease of the effective dislocation glide distance, which results in the "dynamic

14 of 19

Hall–Petch effect", leading to a pronounced increase of strain hardening. In addition, the intragranular twinning evolution including twins' nucleation, propagation and growth has a significant influence on the strain hardening [59], which needs to be investigated in-depth in the further study. The mechanism is given as follows. Twins are assumed to nucleate at grain boundaries, and then propagate rapidly across the grain to form twin bands. At the end of propagation stage, the formed twin bands grow with further deformation. It is noted that stress relaxation appears during propagation stage immediately after twin nucleation and a linear strain hardening during twin growth process would occur [60]. The activity of the slip and twinning systems was performed to investigate the individual contribution of slip and twinning to hardening, respectively. All the slip and twinning systems in the FCC-type TWIP steels are shown in Table 3.

Deformation Mechanism	Symbol	Plane	Direction	Symbol	Plane	Direction
	a ₁	(111)	$\left[01\overline{1}\right]$	b_1	$(\overline{11}1)$	011
	a ₂	(111)	$\overline{101}$	b ₂	$(\overline{11}1)$	[101]
Slin systems	a ₃	(111)	$[1\overline{1}0]$	b ₃	$(\overline{11}1)$	$\overline{110}$
Shp systems	c ₁	$(\bar{1}11)$	$\left[01\overline{1}\right]$	d_1	$(1\overline{1}1)$	$\left[0\overline{11} \right]$
	c ₂	$(\bar{1}11)$	[101]	d2	$(1\overline{1}1)$	$\left[\overline{1}01\right]$
	c ₃	$(\overline{1}11)$	$\left[\overline{11}0\right]$	d ₃	$(1\overline{1}1)$	[110]
	t ₁	(111)	[112]	u ₁	$(\overline{11}1)$	[112]
	t ₂	(111)	211	u ₂	$(\overline{11}1)$	$2\overline{1}1$
Twinning	t ₃	(111)	[1 <u>2</u> 1]	u ₃	$(\overline{11}1)$	<u>[</u> 121]
systems	\mathbf{v}_1	$(\bar{1}11)$	[211]	w_1	$(1\overline{1}1)$	[121]
	v_2	$(\overline{1}11)$	$[12\overline{1}]$	w2	$(1\overline{1}1)$	$21\overline{1}$
	v_3	$(\overline{1}11)$	$\begin{bmatrix} 1\overline{1}2 \end{bmatrix}$	w3	$(1\overline{1}1)$	$\left[\overline{1}12\right]$

Table 3. Twelve slip systems and twelve twinning systems of TWIP (twinning-induced-plasticity) steel.

As shown in Figure 13a, it could be observed that there is symmetric slip systems activation since the resolved shear stress of each slip systems meets the critical value during the tensile deformation. However, with the increase of strain up to about 0.3, the magnitude of slip activity of the slip systems designated as d_1 , a_1 and b_1 remains at a low level. In Figure 13b, it is noted that the twinning systems denoted as v_2 , v_3 , u_1 , u_3 , t_1 and w_3 play a dominative role in hardening evolution, and the hardening is attributed to the fact that it is the twinning boundaries of system that impedes the movement of the dislocations slip and results in the dislocations pile-up, leading to an increasing hardening effect.



Figure 13. (**a**) Active slip systems; and (**b**) twinning systems of the testing sample predicted by simulation with the engineering strain of 0.4.

4.2. Effect of Twinning on Crystal Orientation

The influence of slip and twinning on hardening was investigated and demonstrated that twinning has a larger effect on overall hardening. To determine whether microstructural evolution such as the change of crystallographic orientation is influenced by twinning, a comparison of PF plots predicted by CPFE model without twinning and considering the effect of twinning is given in Figure 14. It is noted that with twinning effect, the scattered orientations in the (111), (110) and (100) PFs obtained from CPFE model considering only slip rotated 90° clockwisely. The occurrence of twinning induced crystals reorientations is shown in Figure 14b. A distinct texture occurred is also shown in the figure. In TWIP steels, deformation twinning appears to transform the Cu component into the Brass-type one. Through the thickness addition of nano-twins, the accumulation of the twin volume fraction occurs. This contribution of twinning to crystallographic texture evolution stems from the effect of twins on the {111} <110>-type slip [10]. In turn, the developments of Cu and Goss components favor twinning. Additionally, twinning also affects the texture development through the generation of new orientations. Therefore, to make a precise prediction of texture evolution, it is essential to introduce twinning into CPFE modeling since twinning has a significant influence on texture evolution.



Figure 14. Comparison of PF plots obtained from CPFE model: (**a**) without twinning; and (**b**) considering the effect of twinning at the strain of 0.4.

4.3. Evolution of Texture Components

As is well known, the anisotropy associated with texture components consisting of Cu and Brass components, influenced by the deformation twinning evolution, plays a significant role in the plastic processing via texture hardening [61]. With the increasing tensile deformation at room temperature, texture components would change significantly due to the evolution of twinning and crystal orientations. To investigate the stability of texture, component evolution could provide a basis for predicting the anisotropy of Fe-Mn-Si-Al TWIP steel. The simulated textures are presented in terms of $\phi_2 = 45^\circ$ sections of the ODFs in the space of Euler angles (ϕ_1 , Φ) $\leq 90^\circ$ via the proposed CPFE model. The final texture components of the samples after uniaxial tension test are shown in the Figure 15. In the ODF plots, it is noted that the strong A and Brass components along the α -fiber could be seen in the simulation results at the strain of 0.05, as shown in Figures 5 and 15. However, only the Brass texture component along the α -fiber is found at the strain of about 0.4, since the Cu orientation rotates to Goss through Cu twin, and finally leads to an increasing of B orientation with the straining. The Goss, Brass and A orientations are dramatically influenced by

twinning formation and its evolution. In the ODF plots of each strain, the ϕ_2 section at 45° exposes a strong Copper component along the τ -fiber, which indicates that the Copper texture is the major part among the deformation textures. Consequently, this CPFE model prediction captures the changing characteristics of the textures named A, Brass and Copper components in measurement and this prediction is similar to those reported previously for the Fe-24Mn-3Al-2Si-1Ni-0.06C TWIP steels [23]. Furthermore, the γ -fiber <111>//ND, with relatively low intensity about 3.0, could be observed in simulation at the strain of 0.1 but disappear with the tensile strain up to 0.4. Thus, this weak γ -fiber could be ignored in the analysis of texture evolution and, further, its influence seems little during the forming process [62]. With the given crystal orientations, the CPFE model describes the main texture components observed in the experimental results although the grain numbers are limited to represent the complete textures. Furthermore, to simulate and predict the anisotropy under uniaxial tension via the texture evolution more precisely, a complex polycrystalline structure with realistic grain properties including grain boundaries must be incorporated in the CPFE simulations.



Figure 15. Constant ODFs ($\phi_2 = 45^\circ$) sections predicted by the CPFE model.

5. Conclusions

By using SEM-based EBSD technique and CPFE model, the characteristics of twinning nucleation and its influence on hardening behavior and crystallographic texture evolution of the Fe-Mn-Si-Al TWIP steels in uniaxial tensile deformation were investigated. The following concluding remarks can be drawn:

- 1. The formation of HAGBs detected by intergranular misorientation distribution could promote the deformation twin lamella nucleation for a FCC-type TWIP steel in uniaxial tensile deformation.
- 2. Twinning promotes the crystal orientation rotation but has less impact on the intensity of crystal distribution compared with no twinning effect. Furthermore, the texture components including the Goss, S and A orientations show a stable volume fraction, while the Cu orientation shifted towards Brass orientation.
- 3. The strain hardening of the studied TWIP steel is dominated by the combined influences of dynamic Hall–Petch effect at the initiation of deformation twinning and texture hardening when the twin volume fraction reaches the saturated value.

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