Postprint: Twinning-Coupled Plastic Deformation Behavior of Polycrystalline TWIP Steel

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Abstract

Based on an established single-crystal plasticity model, a polycrystalline plasticity model for twinning-induced plasticity (TWIP) steel coupled with twinning was developed. The model employs finite-element polycrystalline homogenization to handle geometric compatibility and stress equilibrium conditions between adjacent grains, obtains the relationship between single-crystal and polycrystalline state variables, and develops a computational program based on ABAQUS/UMAT. EBSD was used to investigate the texture evolution of TWIP steel at tensile strains of 0.27 and 0.6, and the model was validated against stress-strain behavior and texture evolution. Using this constitutive model, finite-element models for three simple loading conditions—tension, compression, and torsion—were established respectively, and the macroscopic mechanical responses and texture evolution patterns under different deformation conditions were analyzed. The results show that: during tensile deformation, strain hardening and texture density level increase with strain; during compression, the texture type changes with increasing strain, but the texture density level remains essentially unchanged; whereas during torsion, when the torsional strain is small, virtually no texture forms, and as the strain increases, texture gradually becomes apparent. This is because at small deformations, the internal deformation of the cylinder along the radial direction is small, hence the texture is not pronounced.

Full Text

Investigation of Plastic Deformation Behavior in Polycrystalline TWIP Steel with Coupled Twinning

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Abstract

Twinning induced plasticity (TWIP) steel exhibits high strength and exceptional plasticity due to extensive twin formation under mechanical loading, with ultimate tensile strength and elongation to failure ductility values reaching as high as 5$×10^{4}$ MPa·%, providing a new option for lightweight and safety-enhanced automotive design. Generally, metallic materials exhibit anisotropic behavior after deformation, primarily due to the formation of deformation textures during plastic deformation. The deformation mechanisms responsible for this high strain hardening are related to strain-induced microstructural changes dominated by slip and twinning. Different deformation mechanisms can be activated at various stages of deformation, strongly influencing the stress-strain response and microstructure evolution. In this work, to predict texture evolution under different loading conditions and understand these two deformation mechanisms, a polycrystalline plasticity constitutive model for TWIP steel coupling slip and twinning was developed based on crystal plasticity theory and a single-crystal plasticity constitutive model. A polycrystal homogenization method was employed to maintain geometric compatibility and stress equilibrium between adjacent grains, connecting the state variables of single crystals and polycrystals. The model was then implemented and programmed on the ABAQUS/UMAT platform. Texture evolution was obtained by EBSD at strains of 0.27 and 0.60. Finite element models of tensile, compression, and torsion processes were built using the constitutive model, and the mechanical response and texture evolution during plastic deformation of TWIP steel were analyzed. The results show that during tensile deformation, strain hardening and texture density increase with strain. During compression, texture types change with increasing strain, but texture density remains essentially unchanged. During torsion, no obvious texture forms at small torsional strains; as strain increases, texture gradually emerges because at small deformations, the internal deformation along the radial direction of the cylinder is minimal, resulting in indistinct texture.

Keywords: TWIP steel, crystal plasticity, polycrystal homogenization, texture prediction, plastic deformation

1. Experimental Methods

The TWIP steel polycrystalline material used in this work had a nominal composition of Fe-22Mn-0.6C (mass fraction, %). The raw material was melted in an electromagnetic induction furnace under Ar atmosphere protection, cast into

slabs, hot-rolled to 3.5 mm, then cold-rolled to 1.5 mm. The material was annealed in an SRJX-8-13 box resistance furnace at 800 °C for 75 minutes. After multi-pass rolling on a two-roll cold rolling mill, the thickness was reduced to 1 mm, followed by final rolling on a four-roll cold rolling mill to obtain a 0.5 mm thick TWIP steel sheet. To eliminate the initial rolling texture, the TWIP steel sheet underwent homogenization annealing at 800 °C for 240 s [24].

To investigate the stress-strain characteristics and texture evolution of TWIP steel polycrystals under different deformation conditions, samples were taken from the annealed sheet along the rolling direction. Two groups of tensile tests with different strain levels were conducted on an MTS810 material testing machine at a tensile rate of 8 mm/min. The first group was stretched to a true strain of 0.27, while the second group was stretched to fracture, achieving a true strain of 0.60. The undeformed sample and the two deformed groups were then sectioned for metallographic grinding and electrolytic polishing, and EBSD was employed to observe texture evolution.

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2. Polycrystalline Plasticity Constitutive Model

2.1 Homogenization Method for Polycrystalline Plasticity The single-crystal plasticity constitutive relationship presented in reference [9] analyzed the evolution of slip and twinning systems during single-crystal plastic deformation. By introducing a saturation value for twin volume fraction, the model revealed the evolution of twin volume within single crystals and the influence of twinning on dislocation slip. The hardening moduli for slip and twinning can be characterized as follows [9]:

f^{β} represents the twin volume fraction of the b-th twinning system.

While the above model describes the strain hardening and evolution characteristics of each twinning and slip system during single-crystal plastic deformation of TWIP steel, actual metallic materials are predominantly polycrystalline. Therefore, polycrystal homogenization is required to establish relationships between single-crystal and polycrystal state variables, ensuring that two adjacent crystals satisfy geometric compatibility and stress equilibrium conditions.

Roters et al. [25] proposed a finite element homogenization model based on continuum theory, assuming that one element represents one crystal, with the stress response of material points determined by the response of individual crystals. To distinguish single-crystal variables from polycrystal variables in reference [9], polycrystal variables are denoted with an overbar ("—") unless otherwise specified.

According to continuum large deformation theory, the reference configuration of polycrystal material points is determined by the initial state. After applying external loads, the macroscopic plastic deformation gradient of the polycrystal [25] is:

$\bar{F} = \nabla x$ is the macroscopic plastic deformation gradient, representing the sum of elastic and plastic deformation gradients of the polycrystal; x denotes the position vector from the coordinate origin to the material point; y represents the nonlinear deformation of polycrystal material points, which can be decomposed as [26]:

$\bar{F}^{e}\cdot$ is the combined deformation gradient from elastic deformation (lattice distortion) and rigid rotation of the polycrystal, while $\bar{F}^{p}$ is the plastic deformation gradient caused by slip and twinning deformation.

Both the combined deformation gradient from elastic deformation (lattice distortion) and rigid rotation, and the plastic deformation gradient caused by slip and twinning can be expressed as volume averages of the corresponding deformation gradients of all crystals. The superscripts $n+1$ and n represent the current and previous calculation steps, respectively; $\dot{\gamma}^{\alpha}$ is the slip rate of the a-th slip system; D_t is the time increment; h^{α} and s^{α} are the hardening rate and saturation value of slip resistance for the a-th slip system, respectively, which can be expressed as:

h_0^{α} and s_s^{α} represent the hardening rate and slip resistance saturation value before twinning occurs; s_0, c, and b are material hardening parameters.

The relationship between the polycrystal's second Piola-Kirchhoff average stress and $\bar{F}^{e}$ is:

$\bar{T}^{e} = \bar{F}^{e-1}\bar{T}\bar{F}^{e-T}$ is the polycrystal's second Piola-Kirchhoff average stress, representing the volume average of all crystals' second Piola-Kirchhoff stresses; $\bar{F}^{e-1}$ is the inverse matrix of $\bar{F}^{e}$; $\bar{J} = \det(\bar{F}^{e})$ is the determinant of $\bar{F}^{e}$; $\bar{T}$ is the polycrystal's Cauchy average stress, representing the volume average of all crystals' Cauchy stresses; $\bar{F}^{e-T}$ is the inverse matrix of the transpose of $\bar{F}^{e}$.

The relationship between the polycrystal's first Piola-Kirchhoff average stress and $\bar{T}^{e}$ is:

$\bar{P} = \bar{F}^{e}\cdot\bar{T}^{e}$ is the polycrystal's first Piola-Kirchhoff average stress, representing the volume average of all crystals' first Piola-Kirchhoff stresses; P is the single-crystal first Piola-Kirchhoff stress.

In the above homogenization model, each finite element represents one crystal, with element boundaries coinciding with crystal boundaries. Since most finite elements are conforming elements that satisfy geometric compatibility conditions at element boundaries and stress equilibrium in weak form, the geometric compatibility and stress equilibrium conditions between adjacent crystals can be satisfied.

2.2 Numerical Simulation Process for Polycrystalline Plasticity The numerical simulation process for polycrystalline plasticity in this work is illustrated in [Figure 1: see original paper]. Using ABAQUS/UMAT, all crystals were assigned random initial orientations, and material parameters and calcu-

lation parameters were defined for each crystal. The single-crystal plasticity constitutive model was used to calculate state variables for each crystal during deformation, while the polycrystal homogenization method adjusted stress equilibrium and geometric compatibility between adjacent crystals. After calculation, the required state variables were output.

3. Model Validation

3.1 Parameter Determination for the Polycrystalline Plasticity Model Combining the parameter acquisition method from the TWIP steel single-crystal plasticity constitutive model in references [9,10] and using initial trial values with continuous refinement, the material parameters in the constitutive model were determined. The three material constants in the fourth-order elastic tensor C were taken as $C_{11} = 198$ GPa, $C_{12} = 125$ GPa, and $C_{44} = 122$ GPa; the twin volume fraction threshold f_0 was set to 0.2; the reference plastic shear rate $\dot{\gamma}_0$ was set to 0.001 s^{-1} for quasi-static deformation; the rate sensitivity coefficient $m = 0.0074$; the twinning-to-slip resistance ratio $d = 1.16$; other parameters are given in reference [9].

3.2 Finite Element Model for Polycrystalline Tensile Process In this work, the TWIP steel polycrystalline plasticity constitutive model was numerically simulated through secondary development of ABAQUS/UMAT, and a finite element model for the TWIP steel polycrystalline tensile process was established to reproduce the macroscopic stress-strain relationship and texture evolution under uniaxial tension, as shown in [Figure 2: see original paper]. Considering the loading, deformation, and initial texture distribution characteristics within the effective gauge length during actual tensile testing, a characteristic segment within the effective length can be modeled, shown as the red region in [Figure 2a: see original paper], with dimensions of 2.5 mm × 0.25 mm × 1 mm. Due to symmetry characteristics, symmetric constraints were applied on the left end (about the xz-plane) and back surface (about the zy-plane), the bottom surface was constrained in the z-direction, and the top surface was given a positive displacement in the z-direction. To ensure computational convergence, C3D8 elements (three-dimensional 8-node solid elements) were used, with 320 uniformly divided elements, as shown in [Figure 2b: see original paper]. The initial orientation information for a particular crystal is shown in [Figure 2c: see original paper].

[Figure 3a: see original paper] shows the pole figures of TWIP steel polycrystals after annealing treatment without deformation. It can be seen that the annealed TWIP steel exhibits no obvious annealing texture on {100}, {110}, and {111} planes, with relatively uniform and low pole densities and randomly distributed grain orientations. Barbier et al. [27] observed significant texture in their annealed TWIP steel and therefore considered the influence of initial texture on texture evolution during tensile deformation. In this work, the effect of initial

annealing texture on TWIP steel polycrystalline material was neglected, assuming uniform distribution of all grain orientations after annealing treatment. Based on experimental results under initial conditions, random orientation distribution was assigned to all grains, with the resulting texture shown in [Figure 3b: see original paper]. The randomly oriented TWIP steel shows no obvious texture on {100}, {110}, and {111} planes, with randomly distributed grain orientations that exhibit good consistency with the experimental texture under annealed conditions.

3.3 Validation of Macroscopic Stress-Strain Response and Crystal Orientation Combining TWIP steel polycrystalline tensile experiments with the established finite element model for the tensile process, the experimental and simulated results for stress, strain hardening rate, and twin volume fraction evolution with strain were obtained, as shown in [Figure 4: see original paper]. The simulated stress-strain curves show good agreement with experimental results at strains of 0.27 and 0.60. TWIP steel exhibits high strength and excellent ductility, with tensile strength reaching 1200 MPa and elongation at fracture reaching 80%. As strain continuously increases, strain hardening intensifies while the strain hardening rate gradually decreases. Researchers [28,29] used TEM to observe twin distribution in TWIP steel at different tensile deformation levels, finding that twin volume fraction continuously increases with strain. Consistent conclusions were obtained from the simulation results in [Figure 4: see original paper], with twin volume fraction reaching 15% at fracture.

[Figure 5: see original paper] shows experimental and simulated texture and orientation distribution function (ODF) results at true strains of 0.27 and 0.6. It can be seen that texture gradually forms in TWIP steel polycrystals with increasing strain, and texture intensity continuously strengthens. From the experimental and simulated ODF results, {111}<112> and {111}<110> textures are observed after uniaxial tension. At a strain of 0.27, the primary texture is {111}<112> with a density level around 4. At a strain of 0.6, the {111}<112> texture strengthens, while a new {111}<110> texture emerges, both with density levels around 8. Simultaneously, the sharpness of the tensile texture increases with tensile strain. The comparison demonstrates that the model can satisfactorily predict texture evolution and possesses certain reliability for application in actual plastic processing of TWIP steel polycrystalline materials.

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4. Plastic Deformation of TWIP Steel Polycrystals Under Different Loading Conditions

To further analyze the plastic deformation characteristics and texture formation/evolution patterns of TWIP steel polycrystals under different loading conditions, the established polycrystalline plasticity finite element model was applied to numerical simulations of compression and torsion deformation processes. Similar to the tensile deformation finite element model, all mesh elements employed

C3D8 elements. The compression deformation model used the same characteristic segment dimensions (2.5 mm × 0.25 mm × 1 mm) uniformly divided into 320 finite elements. The displacement boundary conditions were identical to the tensile model, with displacement loading applied in the opposite direction to control deformation magnitude. The torsion deformation finite element model used a cylindrical specimen with diameter 1 mm × length 1 mm, freely meshed with 624 finite elements, with one end fixed and torsional deformation applied to the other end to control deformation magnitude through different twist angles.

[Figure 6: see original paper] presents simulated results for stress, hardening rate, and twin volume fraction evolution during compression and torsion. Stress and twin volume fraction gradually increase with strain, while strain hardening rate gradually decreases in both processes. Comparing [Figure 4: see original paper] and [Figure 6: see original paper], under the same deformation magnitude, compression stress is always greater than tensile stress because the tensile strain hardening modulus of TWIP steel polycrystalline material is smaller than the compressive strain hardening modulus [5].

[Figure 7a: see original paper]–[Figure 7d: see original paper] show simulated pole figures and ODFs at compression strains of 0.8 and 1.52 along the rolling direction. The compressed TWIP steel primarily develops brass and A textures, including {110}<112> and {110}<111> textures. At a strain of 0.8, the main texture is {110}<112> with a density level around 3. At a strain of 1.52, the {110}<111> texture strengthens with density levels around 3. Although texture types change with increasing strain, the average density level remains relatively low.

[Figure 7e: see original paper]–[Figure 7h: see original paper] show pole figures and ODFs after torsion about the rolling direction axis. At small torsion magnitudes, almost no texture forms in TWIP steel polycrystals because during cylindrical torsion, material deformation gradually increases along the radial direction. At small deformations, the internal material experiences minimal deformation, leaving the polycrystalline interior near its initial state, thus texture is not obvious. As deformation increases, internal deformation of the polycrystalline material increases and texture becomes more pronounced. In contrast, under tensile and compressive deformation conditions, all crystals deform under external forces, making texture formation more evident even at small deformations.

Conclusions

(1) The model successfully predicted the formation of brass R-type texture during tensile deformation and revealed that the sharpness of tensile texture increases with tensile strain, showing good consistency with experimental results and validating model reliability.

(2) The tensile strain hardening modulus of TWIP steel polycrystalline material is smaller than the compressive strain hardening modulus, resulting in compression stress always exceeding tensile stress under the same deformation conditions. During tensile deformation, the main texture type changes with increasing strain, and the average density level increases. During compressive deformation, although texture types change with strain, the average density level remains essentially unchanged.

(3) During cylindrical torsion, material deformation gradually increases along the radial direction. At small torsional deformations, texture formation is not obvious due to minimal internal deformation. As strain increases, texture gradually becomes more pronounced.

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Note: Figure translations are in progress. See original paper for figures.