Postprint: Simulation Study on Twinning-Coupled Plastic Deformation Behavior of Single-Crystal TWIP Steel

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Based on crystal plasticity theory, a crystal plasticity constitutive model for twinning-induced plasticity (TWIP) steel single crystals coupling slip and twinning mechanisms was established. By introducing the twin volume fraction and its saturation value, the effects of twinning on hardening and slip were considered separately, and the constitutive model was numerically implemented. Through secondary development on the ABAQUS/UMAT platform, it was applied to simulate the mechanical behavior of TWIP steel single crystals with typical orientations under uniaxial loading conditions. The microscopic mechanisms of plastic deformation, activation states of slip systems and twinning systems, and their influence on macroscopic plasticity under different single-crystal orientations were analyzed. Particularly, the abrupt stress change during loading of Brass orientation and S orientation was simulated, reproducing the stress drop phenomenon observed in Cu single crystal experiments. The results show that when the twin volume fraction is small, its effect on strain hardening is minor; as the twin volume fraction increases, its effect on strain hardening becomes increasingly significant; when the twin volume reaches a certain amount, the twin volume reaches saturation, the twinning increment becomes zero, crystal slip transitions, new slip systems are activated, and stress abruptly drops.

Full Text

Preamble

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Modelling of Plastic Deformation Behavior in Single Crystal TWIP Steel with Coupled Twinning

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Abstract

Based on crystal plasticity theory, a crystal plasticity constitutive model for twinning-induced plasticity (TWIP) steel single crystals was developed by coupling slip and twinning mechanisms. By introducing the twin volume fraction and its saturation value, the model separately considers the effects of twinning on hardening and slip, and the constitutive model was numerically implemented. Through secondary development on the ABAQUS/UMAT platform, the model was applied to simulate the mechanical behavior of TWIP steel single crystals with typical orientations under uniaxial loading conditions. The microscopic mechanisms of plastic deformation in single crystals with different orientations were analyzed, including the activation states of slip and twinning systems and their influence on macroscopic plasticity. In particular, the simulated stress jumps during loading of Brass and S orientations reproduce the stress drop phenomenon observed in copper single crystal experiments. The results show that when the twin volume fraction is small, its effect on strain hardening is negligible; as the twin volume fraction increases, its influence on strain hardening becomes gradually significant. When the twin volume reaches a certain amount, the twin volume saturates, the twinning increment becomes zero, crystal slip reorients, new slip systems activate, and stress suddenly drops.

KEY WORDS TWIP steel; crystal plasticity; slip; twinning; constitutive model

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Introduction

Modern automotive development focuses on energy efficiency and safety improvement. Statistics show that for every 1% reduction in vehicle weight, fuel consumption decreases by 0.6%-1%. Therefore, vehicle weight reduction (lightweighting) represents an important pathway for reducing fuel consumption and environmental protection [?]. Grassel et al. [?, ?] discovered that twinning-induced plasticity (TWIP) steel exhibits not only high tensile strength and high hardening rates, but also excellent ductility, toughness, and formability. Particularly noteworthy is that its product of ultimate tensile strength and elongation (strength-ductility product) can exceed 50,000 MPa・%, which is 4-5 times that of traditional interstitial-free (IF) steel and martensitic steel, and twice that of transformation-induced plasticity (TRIP) steel. Consequently, TWIP steel can maintain high energy absorption performance and impact resistance even when its thickness is reduced by half [?]. TWIP steel demonstrates high strength and toughness primarily due to the activation and evolution of twinning during plastic deformation and its interaction with slip [?].

Researchers [?, ?, ?] have employed modern microscopic testing techniques to investigate the microstructure of TWIP steel before and after tensile or compression testing, confirming that plastic deformation results from the interaction between twinning and slip. They attempted to further understand the interaction 规律 between twinning and slip through experiments [?, ?], aiming to provide references for qualitatively analyzing the contribution of twinning to macroscopic plastic deformation and for developing coupled theoretical models. However, real-time observation of the evolution of individual twinning and slip systems remains difficult. Some scholars have attempted to describe the twinning-induced plasticity mechanism in TWIP steel using physical models, such as the Johnson-Cook empirical constitutive model [?] and the Zerilli-Armstrong physical model [?]. Although these models can simulate strain hardening phenomena after twinning occurs, they cannot track the evolution of twin volume fraction nor explain the influence of twinning on slip. Bouaziz [?, ?] established a work hardening model for TWIP steel using a series of differential equations based on dislocation dynamics. Subsequently, our research group [?] also developed a physical constitutive model considering slip, twinning, and the effect of twinning on slip to study the influence of twinning and slip on macroscopic deformation. These models can analyze the relationship between twin volume fraction and dislocation density evolution, showing good agreement with experimental results, but they cannot fully reflect the evolution of individual twinning and slip systems or the influence of twinning on dislocation slip.

Crystal plasticity theory effectively describes texture evolution during plastic deformation from a mesoscopic perspective, serving as a bridge between macroscopic continuum mechanics and microscopic theory. Therefore, applying crystal plasticity theory to dislocation slip and twinning deformation mechanisms has become a research hotspot in recent years [?]. Classical plasticity theory was established by Taylor [?], Rice [?] provided a more rigorous mathematical description of crystal plasticity theory, and Asaro and Needleman [?] as well as Peirce et al. [?] experimentally validated their theoretical analysis methods. Classical crystal plasticity theory attributes plastic deformation solely to slip mechanisms; however, twinning exists widely as a plastic deformation mechanism. To better describe its influence on macroscopic mechanical behavior, Chin et al. [?] first explored coupling twinning mechanisms into crystal plasticity models. Subsequently, Houtte [?] proposed the PTR (predominant twin reorientation) method, which tracks the total twin volume fraction and reorients the entire grain when a certain random value is reached. Choi et al. [?] modified the PTR method based on experimental observations. Tome et al. [?] proposed the VFT (volume fraction transfer) model and applied it to viscoplastic self-consistent models using a weighted grain orientation approach. In crystal plasticity research, most scholars focus on establishing polycrystalline models using homogenization methods and their correlation with macroscopic mechanical behavior. However, Niewczas et al. [?] observed stress 突变 phenomena in single crystal Cu loading experiments at 4.2 K. Polycrystalline homogenization models consider the effects of grain boundaries, phase boundaries, twin boundaries, and grain orientations in real materials, where macroscopic deformation mechanisms tend to become homogeneous, making it difficult to directly explain the deformation mechanisms causing such 突变 phenomena in single crystal loading processes.

This work considers the characteristics of slip and twinning-induced plasticity in TWIP steel, establishes a crystal plasticity constitutive model for TWIP steel coupling twinning based on crystal plasticity theory, performs numerical implementation and secondary development based on ABAQUS/UMAT. Considering the crystallographic features of TWIP steel, the material parameters required for the single crystal plasticity model are determined. A single crystal plastic finite element model under uniaxial loading conditions is established to analyze the evolution of twinning and slip under different Euler angle loading conditions and their influence on macroscopic deformation behavior, thereby explaining the effects of both mechanisms on TWIP steel plastic deformation.

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1. Theoretical Framework

1.1 Slip and Twinning Deformation Mechanisms in TWIP Steel

TWIP steel has a single stable austenitic microstructure at room temperature. Deformation twins appear during plastic deformation, with the process involving the combined action of slip and twinning mechanisms [?]. Under shear stress, dislocations glide along slip planes. When slip is obstructed, dislocation pile-ups cause stress concentration, making further slip difficult. Simultaneously, during this process, the crystal undergoes twinning deformation along specific twinning directions and planes, with twin volume gradually increasing. When the twin volume fraction reaches a certain level, the crystal orientation changes, transforming originally unfavorable slip orientations into new favorable ones, thereby further activating slip. The alternating progression of twinning and slip enables TWIP steel to achieve excellent strength and ductility [?].

1.2 Kinematic Description Coupling Twinning

Crystal plasticity theory considers slip as the primary pathway for plastic deformation, with deformation accomplished through dislocation glide and crystal rotation [?]. To account for the influence of twinning on the deformation gradient in TWIP steel, twinning is introduced into the multiplicative decomposition of the deformation gradient, which can be decomposed as follows [?]:

$$F = F_e \cdot F_p$$

where F_e represents the combination of elastic deformation (lattice distortion) and rigid rotation, and F_p represents the plastic strain caused by crystal slip and twinning, as shown in Figure 1 [Figure 1: see original paper].

The plastic velocity gradient $L_{p,0}$ defined in the initial configuration is:

$$L_{p,0} = \dot{F}_p \cdot F_p^{-1} = \sum_{\alpha=1}^{a} \dot{\gamma}^{\alpha} S^{\alpha} + \sum_{\beta=1}^{b} \dot{f}^{\beta} \gamma^{\beta} S^{\beta}$$

where a and b are the numbers of slip and twinning systems, respectively, $\dot{\gamma}^{\alpha}$ is the slip rate on slip system α, $\dot{f}^{\beta}$ is the rate of change of twin volume fraction, and γ^{β} is the twinning shear strain, which is a constant. S^{α} and S^{β} are the Schmid tensors for slip and twinning systems, respectively:

$$S^{\alpha} = m^{\alpha} \otimes n^{\alpha}, \quad S^{\beta} = m^{\beta} \otimes n^{\beta}$$

where $\otimes$ denotes the tensor product; m^{α} and n^{α} are the slip direction and slip plane normal in the initial configuration for the α-th slip system; m^{β} and n^{β} are the twinning direction and twinning plane normal in the initial configuration for the β-th twinning system.

1.3 Dynamic Description

According to crystal plasticity theory, the elastic strain tensor E_e can be obtained from the strain gradient [?]:

$$E_e = \frac{1}{2}(F_e^T \cdot F_e - I)$$

where F_e^T is the transpose of F_e, and I is the identity tensor.

The second Piola-Kirchhoff stress T, defined in the intermediate configuration and work-conjugate to E_e, is expressed as [**?**]:

$$T = \det(F_e) F_e^{-1} \cdot \sigma \cdot F_e^{-T}$$

where F_e^{-1} is the inverse of F_e, σ is the Cauchy stress, F_e^{-T} is the inverse of the transpose of F_e, and $\det(F_e)$ is the determinant of F_e.

In typical single crystals, elastic strain values are small, and the elastic stress T can be expressed as a linear function of strain:

$$T = C : E_e$$

where ":" denotes the double dot product, and C is the fourth-order elasticity tensor, which is a constant material matrix.

According to Schmid' s law, the resolved shear stress τ^α on the α-th slip system is:

$$\tau^\alpha = T : S^\alpha$$

When the resolved shear stress τ^α on a slip system exceeds its critical value, the slip system activates. Therefore, Equation (9) can be used to determine whether a slip system is active. For crystal plasticity models, $\dot{\gamma}^\alpha$ can be directly obtained from the resolved shear stress, thereby avoiding uncertainties associated with determining slip system activation [**?**]:

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

where $\dot{\gamma}_0$ is the reference plastic shear rate, s^α is the slip resistance, and m is the rate sensitivity coefficient reflecting material behavior. When $m \to 0$, the rate-dependent model approximates a rate-independent model.

From Equation (1), the expression for the velocity gradient L can be obtained:

$$L = \dot{F} \cdot F^{-1}$$

For twinning, the rate of change of twin volume fraction $\dot{f}^\beta$ can be expressed as [**?**]:

$$\dot{f}^\beta = \frac{\dot{\gamma}^\beta}{\gamma^\beta} = \frac{\dot{\gamma}_0}{\gamma^\beta} \left| \frac{\tau^\beta}{s^\beta} \right|^{1/m} \quad \text{for} \quad \tau^\beta > 0$$

$$\dot{f}^{\beta} = 0 \quad \text{for} \quad \tau^{\beta} \leq 0$$

where τ^{β} is the twinning shear stress on the β-th twinning system, and s^{β} is the twinning resistance.

1.4 Characterization of Hardening Moduli for Slip and Twinning

Based on studies of α-Ti alloys, Kalidindi [**?**] and Wu et al. [**?**, **?**] focused on the effect of twinning on slip while ignoring other hardening contributions, concluding that twinning resistance is proportional to slip resistance during deformation. This conclusion is applied in the present work through the crystal plasticity model in the following form:

$$s^{\alpha}_{n+1} = s^{\alpha}_{n} + \dot{s}^{\alpha}\Delta t$$

where s^{α}_{n+1} is the slip resistance at step $n+1$, $\dot{s}^{\alpha}$ is the hardening rate, and Δt is the time increment. The hardening rate $\dot{s}^{\alpha}$ and slip resistance saturation value s^{α}_{s} can be expressed as:

$$\dot{s}^{\alpha} = \sum_{\beta=1}^{a} h^{\alpha\beta}|\dot{\gamma}^{\beta}| + \sum_{\beta=1}^{b} h^{\alpha\beta}|\dot{f}^{\beta}|$$

$$h^{\alpha\beta} = h_0\left(1 - \frac{s^{\alpha}}{s^{\alpha}_{s}}\right)^{c}, \quad s^{\alpha}_{s} = s_{s0}\left(1 + b\sum_{\beta=1}^{b} f^{\beta}\right)$$

where h_0 and s_{s0} are the hardening rate and slip resistance saturation value without twinning, respectively; b and c are material hardening parameters.

1.5 Expression of Twin Volume Fraction and Grain Reorientation Matrix

According to the literature [**?**], the deformation twin volume fraction $f^{\beta}(\tau)$ caused by twinning can be expressed as:

$$f^{\beta}(\tau) = \frac{\Gamma^{\beta}(\tau)}{\gamma^{\beta}}, \quad \Gamma^{\beta}(\tau) = \int_{0}^{\tau} \dot{\gamma}^{\beta}(\zeta)d\zeta$$

where $\Gamma^{\beta}(\tau)$ is the twinning shear strain for each twinning system, τ and ζ are time variables. In fcc crystals, the twinning shear strain $\gamma^{\beta} = 0.707$ is a fixed value. $f(\tau)$ is the cumulative deformation volume fraction across all twinning systems, i.e., $f(\tau) = \sum_{\beta=1}^{b} f^{\beta}(\tau)$. For a hypothetical reorientation threshold δ, when $f(\tau) > \delta$, the twin completely replaces the parent grain, and the crystal orientation after twinning reorientation becomes:

$$e_{tw} = R \cdot e_{mt}$$

where e_{tw} is the crystal orientation matrix after twinning reorientation, R is the reorientation matrix, and e_{mt} is the crystal orientation matrix of the untwinned parent grain.

Simultaneously, after reorientation, the twin volume fraction reaches its saturation value, twinning ceases within the grain, the Schmid factor is recalculated, and slip system activation is determined based on the new Schmid factor.

The grain reorients according to the twinning system with the maximum twin volume fraction. The reorientation matrix R is expressed as:

$$R = I - 2n \otimes n$$

where n represents the plane normal unit vector of the twinning system with the maximum twin volume fraction.

2. Simulation and Results

2.1 Constitutive Parameters and Finite Element Model for Single Crystal Plasticity with Coupled Twinning

Based on crystal plasticity theory, using the second Piola-Kirchhoff stress and slip resistance as independent variables, the fully implicit numerical integration procedure was derived, and the crystal plasticity constitutive equations with coupled twinning were numerically implemented. By combining crystal plasticity theory with finite element software, secondary development was performed on the ABAQUS/UMAT platform to establish a finite element platform for single crystal plasticity with coupled twinning.

Considering the crystallographic features of TWIP steel, the slip planes and slip directions for the 12 slip systems and the twinning planes and twinning directions for the 12 twinning systems of fcc crystals can be specified, as shown in Tables 1 and 2 . Based on literature [**?**, **?**, **?**, **?**, **?**] and through iterative refinement of material parameters using trial values, the following parameters were obtained for twinning-activated conditions: slip hardening rate $h_s = 300$ MPa, slip resistance saturation value $s_{s0} = 300$ MPa, initial slip deformation resistance $s_{0,\alpha} = 90$ MPa for slip system α, initial twinning deformation resistance $s_{0,\beta} = 104$ MPa for twinning system β, with material parameters $s = 100$ MPa, $b = 2$, and $c = 20$.

To apply the established single crystal plasticity model to describe the roles of various deformation mechanisms and their influence on macroscopic mechanical properties, a finite element model of a TWIP steel single crystal cube under uniaxial loading was developed based on the established model and the secondary development platform. The schematic diagram is shown in Figure 2 [Figure 2: see original paper]. The external load F_w acts in the Z-direction of the initial Cartesian coordinate system, while the grain orientation is defined by the grain reference coordinate system X', Y', Z'. The reference coordinate system forms a certain angle with the initial coordinate system, meaning the loading direction corresponds to a rotation of the cubic crystal coordinate system about the origin by an Euler angle (ψ, θ, ϕ), creating crystals with different orientations. To analyze the influence of different loading conditions on the single crystal plastic deformation process, typical Euler angles were selected for loading simulations.

2.2 Twinning-Induced Macroscopic Plasticity and Hardening Effects

To analyze the influence of twinning on macroscopic plastic deformation and strain hardening, the evolution of stress-strain curves and twin volume fraction was simulated under a loading rate of 0.001 s^{-1}. Since orientation distributions only vary near orientation lines in orientation space during plastic deformation, the tensile results for Cu orientation with Euler angles $(90°, 35°, 45°)$ and Gauss orientation with Euler angles $(0°, 45°, 0°)$ were simulated, as shown in Figure 3 [Figure 3: see original paper]. The results show that the stress for the $(90°, 35°, 45°)$ orientation becomes significantly higher than that for the $(0°, 45°, 0°)$ orientation after strain reaches 0.15. To explain this phenomenon, the twinning shear strain $\Gamma^\beta(\tau)$ and twin volume fraction f^β were further analyzed for both cases. According to Equations (13) and (14), when the twinning shear strain is small, the twin volume fraction is also small due to their proportional relationship, and the effect of twin volume fraction on strain hardening rate h^α is not significant because of parameter b. However, when $\Gamma^\beta(\tau)$ exceeds a certain value, its influence on strain hardening becomes pronounced. In this work, this critical value is approximately 0.08. When the twinning shear strain $\Gamma^\beta(\tau)$ exceeds 0.08, the influence on hardening rate h^α becomes increasingly significant. Moreover, larger twinning shear strain $\Gamma^\beta(\tau)$ leads to larger twin volume fraction f^β, greater hardening modulus, and more pronounced strain hardening. Consequently, the stress for the $(90°, 35°, 45°)$ orientation is significantly higher than that for the $(0°, 45°, 0°)$ orientation.

2.3 Twinning Activation Evolution Conditions and Its Effect on Slip

Niewczas et al. [?] attributed stress jump phenomena to the influence of twinning on slip, but did not specify the contribution values of individual twinning systems or their influence on macroscopic plastic deformation. Moreover, such stress jump phenomena do not typically occur in general polycrystalline plastic deformation. Our research group previously obtained consistent results with literature [?] by simulating copper tensile deformation using a coupled twinning constitutive model with single crystal parameters. To examine whether the TWIP steel single crystal model can explain this phenomenon, this work analyzed the causes of this deformation process and the influence of twinning activation evolution on slip. Two loading cases were selected: Brass orientation with Euler angles $(35°, 45°, 0°)$ and S orientation with Euler angles $(59°, 37°, 63°)$. The stress-strain curves, twin volume fraction evolution, shear amounts for each slip and twinning system, and the evolution of slip and twinning resistances are shown in Figures 4 [Figure 4: see original paper]–6 [Figure 6: see original paper].

As shown in Figure 4 [Figure 4: see original paper], sudden stress drops occur in the stress-strain curves at strains of approximately 0.42 and 0.30 for Euler angles $(35°, 45°, 0°)$ and $(59°, 37°, 63°)$, respectively. Using the loading evolution for the $(35°, 45°, 0°)$ orientation as an example, the states of slip and twinning systems and the influence of twinning on slip were analyzed. The evolution of slip and twinning increments with strain for this orientation is shown in Figures 5 [Figure 5: see original paper] and 6 [Figure 6: see original paper]. The results indicate that this orientation favors activation of twinning systems $t3$ and $u2$, which activate following the initiation of slip systems $a3$ and $b2$, with twinning increments gradually increasing. When strain reaches approximately 0.42, the twin volume fraction f^{β} reaches the set critical value of 0.4, at which point the crystal undergoes reorientation, causing new slip systems $d2$ and $d3$ to activate. After reorientation, slip proceeds on $d2$ and $d3$, while slip continues on the original slip systems. Following reorientation, originally unfavorable slip directions become favorable, resulting in a sudden stress decrease. Additionally, when the twin volume fraction reaches 0.4, the twin volume saturates and the twinning increment abruptly becomes zero. Comparative analysis shows that since the twin volume fraction f^{β} for the $(59°, 37°, 63°)$ orientation reaches 0.4 earlier than that for the $(35°, 45°, 0°)$ orientation, reorientation and stress drop occur first.

Conclusions

1. A single crystal plasticity constitutive model for twinning-induced plasticity (TWIP) steel was established based on crystal plasticity theory. By simulating both slip and twinning mechanisms, the model reflects from a microscopic perspective the influence of coupled twinning on slip mechanisms and its contribution to macroscopic strain hardening.
2. The twin volume fraction was introduced into the hardening modulus expression. When the twin volume fraction is small, its effect on strain hardening can be neglected; as the twin volume fraction increases, its influence on strain hardening becomes significant.
3. The simulated stress jumps for Brass and S orientations match the stress drop phenomenon observed in single crystal Cu experiments. When the twin volume fraction reaches a certain value, it causes crystal slip reorientation and activation of new slip systems, reflecting how the coupling of both mechanisms influences macroscopic mechanical properties.

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