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

Authors: Sun Zhaoyang, Guo Xiangru, Huang Jie, Guo Ning, Wang Shanwei, Yang Jing

Date: 2016-11-04T00:00:00+00:00

Abstract

Based on crystal plasticity theory, a crystal plasticity constitutive model for twinning-induced plasticity (TWIP) steel single crystals was developed, coupling slip and twinning mechanisms. The model separately considers the effects of twinning on hardening and slip by introducing the twin volume fraction and its saturation value. The constitutive model was numerically implemented and further developed on the ABAQUS/UMAT platform, and applied to simulate the mechanical behavior of TWIP steel single crystals with typical orientations under uniaxial loading conditions. The analysis investigated the microscopic mechanisms of plastic deformation, the activation states of slip and twinning systems, and their influence on macroscopic plasticity for different single crystal orientations. In particular, the simulation captured stress jumps during the loading process for Brass and S orientations, which reproduces the stress drop phenomenon observed in Cu single crystal experiments. Simulation results indicate 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 level, the twin volume saturates, the twinning increment becomes zero, crystal slip transitions, new slip systems are activated, and a stress drop occurs.

Full Text

Modelling of Plastic Deformation on Coupling Twinning of Single Crystal TWIP Steel

Sun Chaoyang, Guo Xiangru, Huang Jie, Guo Ning, Wang Shanwei, Yang Jing
School of Mechanical Engineering, University of Science and Technology Beijing,

Beijing 100083
Correspondent: suncy@ustb.edu.cn

Supported by: Joint Fund of National Natural Science Foundation of China and Chinese Academy of Engineering Physics (No. U1330121), National Natural Science Foundation of China (No. 51105029), and Beijing Science Foundation of China (No. 3112019)

Manuscript received: 2014-06-04; in revised form: 2014-10-16

Abstract

Based on crystal plasticity theory, a crystal plasticity constitutive model for twinning-induced plasticity (TWIP) steel single crystal was established 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, and the activation states of slip and twinning systems and their influence on macroscopic plasticity were investigated. In particular, the stress jump phenomenon during the loading process of brass Cu orientation and S orientation was simulated, reproducing the steep stress drop observed in copper single crystal experiments. The results show that when the twin volume fraction is small, its effect on strain hardening can be neglected; as the twin volume fraction increases, its effect becomes gradually significant; when the twin volume reaches a certain level, the twin volume saturates, the twinning increment becomes zero, crystal slip reorients, new slip systems activate, and the stress suddenly drops.

Key words: TWIP steel, crystal plasticity, slip, twinning, constitutive model

---

1. Coupled Twinning TWIP Steel Single Crystal Plastic Constitutive Model

1.1 TWIP Steel Slip and Twinning Deformation Mechanisms

TWIP steel has a single stable austenite microstructure at room temperature, and deformation twins appear during plastic deformation. This process involves the combined action of slip and twinning mechanisms. Under shear stress, dislocations glide along slip planes. When slip is obstructed, dislocation pile-up occurs, causing stress concentration and making further slip difficult. Simultaneously, during this process, the crystal undergoes twinning deformation along specific twinning directions and twinning planes, and the twin volume fraction gradually increases. When the twin volume fraction reaches a certain level, the crystal orientation changes, which can transform 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 plasticity.

1.2 Kinematic Description of Coupled Twinning

Crystal plasticity theory considers slip as the primary pathway for plastic deformation, which is accomplished by dislocation glide and crystal rotation. To account for the effect of twinning on the deformation gradient in TWIP steel, twinning is introduced into the multiplicative decomposition of the deformation gradient. The deformation gradient $\mathbf{F}$ can be decomposed as follows:

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p$$

where $\mathbf{F}_e$ represents the combination of elastic deformation (lattice distortion) and rigid rotation, and $\mathbf{F}_p$ represents the plastic strain caused by crystal slip and twinning, as shown in [Figure 1: see original paper].

From Eq. (1), the expression for the velocity gradient $\mathbf{L}$ can be obtained:

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

The plastic velocity gradient $\mathbf{L}_{p,0}$ defined in the initial configuration is:

$$\mathbf{L}_{p,0} = \sum_{\alpha=1}^{N_s} \dot{\gamma}^{\alpha} \mathbf{S}^{\alpha} + \sum_{\beta=1}^{N_t} \dot{f}^{\beta} \gamma^{\beta} \mathbf{S}^{\beta}$$

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

$$\mathbf{S} = \mathbf{m} \otimes \mathbf{n}$$

where $\otimes$ denotes the tensor product; $\mathbf{m}^{\alpha}$ and $\mathbf{n}^{\alpha}$ are the slip direction and slip plane normal of the α-th slip system in the initial configuration, respectively; and $\mathbf{m}^{\beta}$ and $\mathbf{n}^{\beta}$ are the twin direction and twin plane normal of the β-th twinning system in the initial configuration, respectively.

1.3 Dynamic Description of Coupled Twinning

According to crystal plasticity theory, the elastic strain tensor $\mathbf{E}_e$ can be obtained from the elastic deformation gradient:

$$\mathbf{E}_e = \frac{1}{2}(\mathbf{F}_e^{\mathrm{T}}\mathbf{F}_e - \mathbf{I})$$

The second Piola-Kirchhoff stress $\mathbf{T}_e$, which is work-conjugate with $\mathbf{E}_e$ and defined on the intermediate configuration, is expressed as:

$$\mathbf{T}_e = \det(\mathbf{F}_e)\mathbf{F}_e^{-1}\mathbf{T}\mathbf{F}_e^{-\mathrm{T}}$$

where $\mathbf{F}_e^{-1}$ is the inverse of $\mathbf{F}_e$, $\det \mathbf{F}_e$ is the determinant of $\mathbf{F}_e$, $\mathbf{T}$ is the Cauchy stress, and $\mathbf{F}_e^{-\mathrm{T}}$ is the inverse of the transpose of $\mathbf{F}_e$.

In general single crystals, the elastic strain values are small, and the elastic stress $\mathbf{T}_e$ can be expressed as a linear function of strain:

$$\mathbf{T}_e = \mathbf{C} : \mathbf{E}_e$$

where ":" denotes the double dot product and $\mathbf{C}$ is the fourth-order elasticity tensor, which is a constant material property matrix.

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

$$\tau^\alpha = \mathbf{S}^\alpha : \mathbf{T}_e$$

When the resolved shear stress τ^α on a slip system exceeds its critical value τ_c, the slip system activates, so Eq. (9) can be used to determine whether a slip system is active.

For the crystal plasticity model, $\dot{\gamma}^\alpha$ can be directly obtained from the resolved shear stress, thereby avoiding the uncertainty of determining whether a slip system is active:

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

where $\dot{\gamma}_0$ is the reference plastic shear rate, s^α is the slip resistance, and m reflects the material' s rate sensitivity coefficient. The function $\mathrm{sign}(\tau^\alpha)$ is the sign function, and when $m \to 0$, the rate-dependent model approximates a rate-independent model.

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

$$\dot{f}^{\beta} = \dot{\gamma}_0 \left(\frac{\tau^{\beta}}{s^{\beta}} \right)^{1/m}$$

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 Modulus for Slip and Twinning

Based on studies of -Ti alloys, Kalidindi and Wu et al. focused on the effect of twinning on slip while ignoring other hardening effects, and found that twinning resistance is proportional to slip resistance during deformation. By considering the crystal plasticity model, this conclusion is applied in the present work. The specific form is as follows:

$$s_{n+1}^{\alpha} = s_n^{\alpha} + \dot{s}_h^{\alpha} \Delta t$$

where s_{n+1}^{α} is the slip resistance at the $(n+1)$-th calculation step, n is the step number, Δt is the time increment, $\dot{s}_h^{\alpha}$ and s_s^{α} are the hardening rate and saturation value of slip resistance for the α-th slip system, respectively, which can be expressed as:

$$\dot{s}_h^{\alpha} = \dot{s}_{h0}^{\alpha} \left(1 + \frac{f}{c} \right)^{b}, \quad s_s^{\alpha} = s_{s0}^{\alpha} \left(1 + \frac{f}{c} \right)^{b}$$

where $\dot{s}_{h0}^{\alpha}$ and s_{s0}^{α} are the hardening rate and slip resistance saturation value without twinning, respectively, and p_{rs}, c, and b 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 is expressed as:

$$f_{\beta}(\tau) = \sum_{\beta=1}^{N_t} \int_0^{\tau} |\dot{\gamma}_{\beta}| \, d\zeta$$

where $\dot{\gamma}_{\beta}$ is the twinning shear strain rate of each twinning system, and τ and ζ are time variables. In fcc crystals, the twinning shear strain $f(\tau)$ is the cumulative sum of deformation volume fractions in all twinning systems, i.e., $f(\tau) = \sum_{\beta=1}^{N_t} f_{\beta}(\tau)$. 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:

$$\mathbf{e}_{tw} = \mathbf{R}_{tw}\mathbf{e}_{mt}$$

where $\mathbf{e}_{tw}$ is the crystal orientation matrix after twinning reorientation, $\mathbf{R}_{tw}$ is the twinning reorientation matrix, and $\mathbf{e}_{mt}$ is the crystal orientation matrix of the untwinned parent grain.

Simultaneously, after reorientation, the twin volume fraction reaches its saturation value, no further twinning occurs within the grain, and the Schmid factor is recalculated to determine the activation of slip systems based on the new Schmid factor. The grain reorients according to the direction of the twinning system with the maximum twin volume fraction. The expression for the reorientation matrix $\mathbf{R}_{tw}$ is:

$$\mathbf{R}_{tw} = \mathbf{I} + (\mathbf{g}_{\text{twin}} \otimes \mathbf{g}_{\text{twin}})$$

where $\mathbf{g}_{\text{twin}}$ represents the unit normal vector of the twinning plane with the maximum twin volume fraction, and $\mathbf{I}$ is the identity matrix.

2.1 Coupled Twinning Single Crystal Plastic Constitutive Parameters and Finite Element Model

Based on crystal plasticity theory, a fully implicit numerical integration process was derived using the second Piola-Kirchhoff stress and slip resistance as independent variables, and the coupled twinning crystal plasticity constitutive equations were numerically implemented. The crystal plasticity theory was then combined with finite element software, and a coupled twinning single crystal plastic finite element platform was established through secondary development on the ABAQUS/UMAT platform.

Considering the crystallographic characteristics of TWIP steel, the 12 slip systems' slip planes and slip directions and the 12 twinning systems' twinning planes and twinning directions for fcc crystals can be given, as shown in and . Based on literature [24-28] and by taking some trial values to continuously correct the material parameters in the constitutive model, the following parameters were obtained: slip hardening rate $h_s = 300$ MPa, slip resistance saturation value $s_{s0} = 300$ MPa, initial slip deformation resistance $s_{0,\alpha} = 90$ MPa, initial twinning deformation resistance $s_{0,\beta} = 104.4$ MPa, and material parameters $p_{rs} = 100$ MPa, $b = 2$, and $c = 20$.

To apply the established single crystal plasticity model to describe the role of various deformation mechanisms and their influence on macroscopic mechanical properties, a finite element model of TWIP steel single crystal cube under uniaxial loading was established based on the developed model and the secondary-developed single crystal plasticity finite element platform. The schematic diagram is shown in [Figure 2: see original paper]. The external load F_w acts in the Z-direction of the initial Descartes coordinate system X, Y, Z, while the grain orientation is 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 is formed by rotating 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 analysis to investigate twinning activation, evolution, and their influence on macroscopic mechanical behavior.

2.2 Twinning-Induced Macroscopic Plasticity and Hardening Effects

To analyze the influence of twinning on macroscopic plastic deformation and strain hardening, the evolution laws of stress-strain and twin volume fraction were simulated under a loading rate of 0.001 s ^{1}. Since orientation distribution only changes near the orientation line 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: see original paper].

The results show that the stress for Euler angle $(90°, 35°, 45°)$ becomes significantly greater than that for Euler angle $(0°, 45°, 0°)$ after the strain reaches 0.15. To explain this phenomenon, the twinning shear strain $\Gamma_\beta(\tau)$ and twin volume fraction f_β under the two conditions were further analyzed. According to Eqs. (13) and (14), when the twinning shear strain is small, the twin volume fraction is also small due to the proportional relationship between them, and the effect of twin volume fraction on strain hardening rate $\dot{s}_h^\alpha$ is not obvious due to the influence of b. However, when $\Gamma_\beta(\tau)$ exceeds a certain value, its effect on $\dot{s}_h^\alpha$ becomes significant. In this work, this value is approximately 0.08. When the twinning shear strain $\Gamma_\beta(\tau)$ exceeds 0.08, its influence on $\dot{s}_h^\alpha$ gradually becomes pronounced. Moreover, the larger the twinning shear strain $\Gamma_\beta(\tau)$, the larger the twin volume fraction f_β, and the greater the hardening modulus $\dot{s}_h^\alpha$. Therefore, the stress for the orientation with Euler angles $(90°, 35°, 45°)$ is significantly greater than that for the orientation with Euler angles $(0°, 45°, 0°)$.

2.3 Twinning Activation Evolution Conditions and Its Effect on Slip

Niewczas et al. believed that the stress jump phenomenon is caused by the effect of twinning on slip, but they did not specify the contribution values of each twinning system or their influence on macroscopic plastic deformation. Moreover, this stress jump phenomenon does not generally appear in polycrystalline plastic deformation processes. Our research group used a coupled twinning constitutive model and brass-related parameters to simulate the tensile deformation process of single crystal Cu and obtained results consistent with literature [23]. To examine whether the TWIP steel single crystal model can explain this phenomenon, the causes of this deformation process and the influence of twinning activation evolution on slip were analyzed. This work selected two cases: brass Cu 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 evolution of each slip and twinning system, and evolution of slip resistance and twinning resistance under these two conditions are shown in [FIGURE:4-6].

As can be seen from [Figure 4: see original paper], sudden stress drops appear in the stress-strain curves at strains of approximately 0.42 and 0.3 for Euler angles $(35°, 45°, 0°)$ and $(59°, 37°, 63°)$, respectively. Taking the loading evolution law for Euler angle $(35°, 45°, 0°)$ as an example, to analyze the status of each slip and twinning system and the influence of twinning on slip, the evolution results of the increments of 12 slip systems and 12 twinning systems with strain under this orientation condition are shown in [Figure 5: see original paper] and [Figure 6: see original paper]. It can be observed that this orientation condition favors the activation of twinning systems t3 and u2. After slip systems a3 and b2 are activated, these twinning systems are also activated, and the twinning increment gradually increases. When the strain reaches approximately 0.42, the twin volume fraction f_β reaches the set critical value of 0.4. At this point, the crystal undergoes reorientation, causing new slip systems d2 and d3 to activate. After reorientation, slip begins on d2 and d3 while continuing on the original slip systems. Following reorientation, the originally unfavorable slip direction transforms into a favorable slip direction, resulting in a sudden stress decrease. Simultaneously, when the twin volume fraction reaches 0.4, the twin volume saturates and the twinning increment abruptly becomes zero. Through comparison, since the twin volume fraction f_β for Euler angle $(59°, 37°, 63°)$ reaches 0.4 earlier than that for Euler angle $(35°, 45°, 0°)$, reorientation occurs first, leading to an earlier stress drop.

Conclusions

(1) Based on crystal plasticity theory, a single crystal plastic constitutive model for TWIP steel was established. By simulating both slip and twinning mechanisms, the influence of coupled twinning on slip mechanisms and its contribution to macroscopic strain hardening were reflected at the microscopic level.

(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 ignored; as the twin volume fraction increases, its effect on strain hardening becomes significant.

(3) The simulated stress jumps for brass Cu orientation and S orientation are consistent with the steep 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 the influence of the coupling between the two mechanisms on

macroscopic mechanical properties.

References

[1] Senuma T. ISIJ Int, 2001; 41: 520
[2] Grassel O, Frommeyer G, Derder C, Hofmann H. J Phys IV France, 1997; 5: 383
[3] Grassel O, Kruger L, Frommeyer G, Meyer L W. Int J Plast, 2000; 16: 1391
[4] Tang D, Mi Z L, Chen Y L. Iron Steel, 2005; 4: 1 (唐荻, 米振莉, 陈雨来. 钢铁, 2005; 4: 1)
[5] Grassel O, Kruger L, Frommeyer G, Meyer L W. Int J Plast, 2000; 16: 1394
[6] Frommeyer G, Grassel O. Rev Metall CIT, 1997; 97: 32
[7] Wang X Y. Master Thesis, Northeastern University, Shenyang, 2011 (王祥元. 东北大学硕士学位论文, 沈阳, 2011)
[8] Li W. Master Thesis, Northeastern University, Shenyang, 2006 (李卫. 东北大学硕士学位论文, 沈阳, 2006)
[9] Idrissi H, Renard K, Ryelandt L, Schryvers D, Jacques P J. Acta Mater, 2010; 58: 2476
[10] Gutierrez-Urrutia I, Raabe D. Acta Mater, 2011; 59: 6449
[11] Johnson G R, Cook W H. Eng Fract Mech, 1985; 21: 31
[12] Zerilli F J, Armstrong R W. J Appl Phys, 1987; 61: 1816
[13] Bouaziz O. Scr Mater, 2012; 66: 982
[14] Bouaziz O, Guelton N. Mater Sci Eng, 2001; 319A: 246
[15] Sun C Y, Huang J, Guo N, Yang J. Acta Metall Sin, 2014; 50: 1115 (孙朝阳, 黄杰, 郭宁, 杨竞. 金属学报, 2014; 50: 1115)
[16] Taylor G I. Inst Met, 1938; 62: 307
[17] Rice J R. J Mech Phys Solids, 1971; 19: 433
[18] Asaro R J, Needleman A. Acta Mater, 1985; 33: 923
[19] Peirce D, Asaro R J, Needleman A. Acta Mater, 1982; 30: 1087
[20] Chin G Y. Proc R Soc Lond Ser, 1969; 309A: 433
[21] Houtte V P. Acta Metall, 1978; 26: 591
[22] Choi S H, Shin E S, Seong B S. Acta Mater, 2007; 55: 4181
[23] Tome C N, Lebensohn R A, Kocks U F. Acta Metall Mater, 1991; 39: 2667
[24] Niewczas M, Basinski Z S, Basinski S J, Embury J D. Philos Mag, 2001; 81A: 1121
[25] Cao P, Fang G, Lei L P, Zeng P. Acta Metall Sin, 2007; 43: 913 (曹鹏, 方刚, 雷丽萍, 曾攀. 金属学报, 2007; 43: 913)
[26] Salem A A, Kalidindi S R, Semiatin S L. Acta Mater, 2005; 53: 3495
[27] Kalidindi S R. J Mech Phys Solids, 1998; 46: 267
[28] Van Houtte P, Li S, Seefeldt M, Delannay L. Int J Plast, 2005; 21: 589
[29] Wu X P. PhD Dissertation, Drexel University, 2006
[30] Wu X P, Kalidindi S R, Necker C. Acta Mater, 2007; 55: 42

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

Source: ChinaXiv —Machine translation. Verify with original.