Numerical Modeling of Twinning Induced Plasticity in Austenite based Advanced High Strength Steels

Rashid Khan\textsuperscript{1,*}, Fahad I. Zahedi\textsuperscript{1}, and Ali K. Siddiqui\textsuperscript{1}

Mechanical Engineering Department, College of Engineering, Al Imam Mohammad Ibn Saud Islamic University, Riyadh 11432, Kingdom of Saudi Arabia

Abstract
Advanced manufacturing techniques make it possible to attain large deformation of material in order to obtain required shape of a product. However, one of the main reasons behind their successful implementation is having an optimum combination of strength and formability of a material. The enduring challenge of increasing these two contradictory properties simultaneously is achieved through the invention of Advanced High Strength Steels. Advanced high strength steels cover a vast range of applications, more specifically in aerospace, automotive, and oil industry where large deformation of a material is desired to attain a specified shape and geometry of the product. Austenite based twinning induced plasticity steel lies in the second generation and has excellent strength and formability among the group of advanced high strength steels. The stress assisted phase transformation from austenite to martensite, which is known as twinning, found to be principal reason behind an enhancement of these properties. This work is aimed to investigate an elastic-plastic behavior of an austenite based steel, which undergoes slip and mechanical twinning modes of deformation. Initially, a micromechanical model of twinning induced plasticity is developed using crystal plasticity theory. Then, the developed model is numerically implemented into finite element software ABAQUS through a user-defined material subroutine. Finally, finite element simulations are done for single and polycrystal austenite subjected to combined load. This replicates the complex loading condition which exists in material forming processes like pipe expansion, extrusion, rolling, etc. The variation in stress-strain response, magnitude of shear strain, and volume fraction of twinned martensite are plotted and analyzed.

Keywords: Micromechanical modeling, finite element simulations, twinned martensite, crystal plasticity theory

INTRODUCTION

In most of the applications of metallic materials especially in large deformation problems, strength and ductility are two important properties. Since decades, processes like heat treat-
ment, solid solution strengthening, precipitation hardening etc. are commonly used to enhance one of these two properties. One of the major constraints with these techniques is that an increment in one property is achieved at the expense of the other. The enduring challenge for developing a class of steels where both strength and formability can simultaneously be improved was answered when advanced high strength steels (AHSS) were invented. The enhancement in their properties is achieved by developing more complex microstructure through controlled processes during manufacturing. Twinning based steels show the highest combination of strength and formability among AHSS where the tensile strength reaches up to 1000 MPa while percentage elongation is up to 70% (Tamarelli, 2011). This combination of properties can be achieved through the addition of optimum percentage of Manganese (up to 22%) which significantly reduce stacking fault energy of an alloy. The reduction in stacking fault energy activates twining mode of permanent deformation even at low strain.

Twinning, or more specifically mechanical twinning, is another mode (along with slip) of plastic deformation in crystals, which exists in metallic, non-metallic and even in organic materials. Twinning is a crystal shearing phenomenon where the atomic planes are displaced in a way that it transforms the lattice orientation into a mirror image across a twin or habit or composition plane. The resultant lattice structure is commonly known as twinned crystal (or twinned martensite in case of twinning in face centered cubic austenite to body centered tetragonal martensite). Mechanical twinning plays a vital role in enhancing the properties of TWIP steels. Austenitic steels can exhibit both high strength and ductility due to a particularly high work hardening rate. Among all the possible deformation modes for austenitic steels, Twinning Induced Plasticity (TWIP) has the most beneficial effect on the work-hardening. It is believed that deformation twins increase the work-hardening rate by acting as obstacles for gliding dislocations (Asgari et al., 1997), (Bouaziz et al., 2011). Therefore, a thorough understanding of twinning phenomenon is necessary to estimate its effects on the properties of TWIP steels.

Modeling a twinning phenomenon based on the theory of crystal plasticity finite element method has major practical significance especially in altering the mechanical properties of shape memory alloys (Bhattacharya, 1991), (Wang and Sehitoglu, 2013) and steels that have high strength with excellent forming characteristics (Allain et al., 2004), (Bouaziz, 2012). Other major applications include elastic-plastic deformation behavior of magnesium alloys (Khosravani et al., 2013) and high-Mn austenitic steels (Shiekhelsouk et al., 2009), (Peng et al., 2013) where the stress-strain behavior is also dominantly dependent on twinned martensite volume fraction. In spite of the availability of extensive work, there are still some gaps (especially related to the mechanics and energy based modeling of twinning induced plasticity) which needs to be filled. The main focus of the present work is to develop a kinematic and thermodynamic framework for slip and twinning based crystal plasticity model. Initially, a kinematics of the deformation is defined through the decomposition of deformation gradients. A novel thermodynamic framework is developed to estimate the dissipated energy, Helmholtz free energy, and the driving potentials for slip and twinning mechanisms. The model is then numerically implemented into a finite element software ABAQUS through a user-defined material subroutine. The model is validated through a published experimental result. Finally, finite element simulations are performed for single and polycrystal austenite.

MATHEMATICAL MODELING

A micromechanical model is developed in order to estimate the slip and twin based elastic-plastic deformation of an austenite crystal once subjected to thermo-mechanical load. A mathematical model is formulated by integrating twin deformation theory in the slip based crystal plasticity model. This model would be able to predict the stress-strain behavior of a crystal undergoes slip
Figure 1: Kinematic decomposition of elastic-plastic deformation of single crystal austenite subjected to thermo-mechanical load and twin modes of permanent deformation. A stress-strain constitutive relation is developed through the kinematic decomposition of deformation of an austenite crystal into intermediate configurations.

**Kinematics**

The kinematics of a single crystal based on the finite deformation theory can be expressed using multiplicative decomposition of total deformation gradient proposed by (Lee, 1969) as

\[ F = F^e F^p, \]  

where \( F \) represents the total deformation gradient while \( F^e \) and \( F^p \) are the elastic and plastic deformation gradients. The elastic deformation gradient can further be decomposed into symmetric left stretch tensor \( U^e \) and the orthogonal rotation tensor \( R^e \) i.e. \( F = U^e R^e F^p \). The rotation and plastic deformation gradient tensors can be combined into a plastic rigid rotation tensor \( F^r \) as

\[ F = U^e F^r, \quad F^r = R^e F^p = R^e F^p_s F^p_t, \]  

where plastic deformation gradient \( F^p \) is disintegrated into plastic deformation gradient due to slip \( F^p_s \) and twinning \( F^p_t \). The phenomenon of elastic-plastic deformation of a crystal which involves two modes, slip and twin, of plastic deformation can be further elaborated using a kinematic decomposition of the whole mechanism, as shown in Figure 1.

Let \( B_0 \) and \( B_f \) represent the reference (undeformed) and current (deformed) configurations of a material point in a FCC-austenite crystal. The decomposition of total deformation gradient in case of slip and twinned based elastic-plastic deformation of a crystal can be represented by three intermediate states as shown in Figure 1. The configuration \( \widetilde{B}_1 \) represents the plastic deformation due to crystallographic slip, \( \widetilde{B}_2 \) represents twinned based plastic deformation, and \( \widetilde{B}_3 \) represents rigid body rotation. The final deformed state of a material (\( B_f \)) is projected...
from $\tilde{\mathbf{B}}_3$ through stretch tensor $\mathbf{U}^e$. The velocity gradient in the current configuration $\mathbf{B}_f$ can by represented as

$$\mathbf{L} = \dot{\mathbf{F}} \mathbf{F}^{-1} = \dot{\mathbf{U}}^e (\mathbf{U}^e)^{-1} + \mathbf{U}^e \tilde{\mathbf{L}}^* (\mathbf{U}^e)^{-1},$$

(3)

$\tilde{\mathbf{L}}^*$ is the velocity gradient in $\tilde{\mathbf{B}}_3$. The plastic velocity gradient $\mathbf{L}^p$ is given as

$$\mathbf{L}^p = \tilde{\mathbf{L}}_s^p + \mathbf{F}^p_s \tilde{\mathbf{L}}^p (\mathbf{F}^p_s)^{-1} = \sum_{i=1}^{N_{sl}} \tilde{\gamma}^i \mathbf{S}^i + \sum_{i=1}^{N_{tw}} \tilde{\gamma}^i \hat{\mathbf{S}}^i (\mathbf{F}^p_s)^{-1},$$

(4)

$\tilde{\mathbf{L}}_s^p$ and $\tilde{\mathbf{L}}^p$ are the plastic velocity gradients due to slip and twinning, respectively, $\alpha$ represents a slip system, $N_{sl}$ is the total number of slip systems in a crystal, $\tilde{\gamma}^i$ is the plastic shear strain rate. The Schmid orientation tensor $\mathbf{S}^i$ is defined by the dyadic product of slip direction vector $\hat{m}$ and area normal vector of twin plane $\mathbf{n}$. $i$ represents the twin system, $N_t$ is the total number of twin systems, $\tilde{\gamma}^i$ is the plastic shear strain rate of $i$-twin system, $\hat{\mathbf{S}}^i$ is the twin orientation tensor in $\tilde{\mathbf{B}}_2$, expressed by the dyadic product of twin direction vector $\mathbf{m}$ and area normal vector of twin plane $\mathbf{n}$. The mechanical twinning is assumed to occur within the plastically deformed region due to slip. This necessitates the inclusion of respective volume fractions of slip and twinned regions in Eq.(4)

$$\mathbf{L}^p = \left( 1 - \sum_{i=1}^{N_{sl}} v^i \right) \sum_{i=1}^{N_{sl}} \tilde{\gamma}^i \mathbf{S}^i + \sum_{i=1}^{N_{tw}} \tilde{\gamma}^i \hat{\mathbf{S}}^i (\mathbf{F}^p_s)^{-1},$$

(5)

In Eq.(5), $v^i$ represents the volume fraction of $i$-twin system $\tilde{\mathbf{B}}_2$. Similarly, $\tilde{\mathbf{L}}^*$ can be rewritten as

$$\tilde{\mathbf{L}}^* = \tilde{\Phi}^e + \mathbf{R}^e \left[ \left( 1 - \sum_{i=1}^{N_{sl}} v^i \right) \sum_{i=1}^{N_{sl}} \tilde{\gamma}^i \mathbf{S}^i + \sum_{i=1}^{N_{tw}} \tilde{\gamma}^i \hat{\mathbf{S}}^i (\mathbf{F}^p_s)^{-1} \right] (\mathbf{R}^e)^T,$$

(6)

$\tilde{\Phi}^e$ represents spin of the crystal. The Schmid $\mathbf{S}^i$ and twin orientation $\hat{\mathbf{S}}^i$ tensors can be mapped from $\tilde{\mathbf{B}}_2$ to $\tilde{\mathbf{B}}_3$ through forward transformation as: $\mathbf{S}^i = \mathbf{R}^e \mathbf{S}^i (\mathbf{R}^e)^T$, and $\hat{\mathbf{S}}^i = \mathbf{R}^e \hat{\mathbf{S}}^i (\mathbf{R}^e)^T$. Using backward mapping from configurations $\mathbf{B}_f$ to $\tilde{\mathbf{B}}_3$ and Eq.(3), $\tilde{\mathbf{L}}$ can be expressed as

$$\tilde{\mathbf{L}} = (\mathbf{U}^e)^{-1} \mathbf{L} \mathbf{U}^e = (\mathbf{U}^e)^{-1} \mathbf{U}^e + \tilde{\mathbf{L}}^*$$

$$= (\mathbf{U}^e)^{-1} \dot{\mathbf{U}}^e + \tilde{\Phi}^e + \left[ \left( 1 - \sum_{i=1}^{N_{sl}} v^i \right) \sum_{i=1}^{N_{sl}} \tilde{\gamma}^i \mathbf{S}^i + \sum_{i=1}^{N_{tw}} \tilde{\gamma}^i \hat{\mathbf{S}}^i (\mathbf{F}^p_s)^{-1} \right].$$

(7)

The constitutive relation can be written as

$$\mathbf{T}^e = \tilde{\mathbf{C}}^e : \tilde{\mathbf{E}}^e,$$

(8)

$\mathbf{T}^e$ is the second Piola-Kirchhoff stress tensor, $\tilde{\mathbf{C}}^e$ is the equivalent elasticity tensor, and $\tilde{\mathbf{E}}^e$ is the Green strain tensor. The equivalent elasticity tensor is defined as a volume average of untwinned and twinned regions as

$$\tilde{\mathbf{C}}^e = \left( 1 - \sum_{i=1}^{N_{sl}} v^i \right) \tilde{\mathbf{C}}^e + \sum_{i=1}^{N_{tw}} v^i \tilde{\mathbf{C}}^e,$$

(9)

775
where $\widetilde{C}_s$ and $\widetilde{C}_t$ are the elasticity tensors of untwinned and twinned regions, respectively. In elastic-plastic especially large deformation problems related to metals, the elastic contribution to total strain is very small as compared to plastic. Therefore, the crystal plasticity formulation illustrated here is not quite susceptible to stress and strain measures which explains elasticity. Furthermore, the different elasticity tensors for untwinned and twinned regions are included with the intentions of considering the mismatch in the lattice orientations of these regions.

**THERMODYNAMIC FORMULATION**

A thermodynamic framework is developed for deriving constitutive equations of energy dissipation, driving potential, and Helmholtz free energy for elastic-plastic deformation of single and polycrystal FCC-austenite subjected to thermo-mechanical load.

The dissipated energy is the difference of total and internal strain energy of the system and it can be represented as

$$\dot{E}_d = \sigma \dot{F} + \rho_0 \theta \dot{\Pi}_m - \rho_0 \dot{\epsilon} - \nabla \vec{q}. \quad (10)$$

where $\sigma$ is the first Piola-Kirchhoff stress, $\rho_0$ is the density of an austenite, $\theta$ is the temperature, $\dot{\Pi}_m$ is the rate of entropy change due to an external thermal load, $\dot{\epsilon}$ is the rate of internal energy per unit mass, and $\vec{q}$ is the heat flux per unit surface area. The first two terms of Eq.(10) represent the mechanical and thermal load contribution to the total energy, the third term shows the internal energy, and last represents heat loss due to temperature gradient.

The rate of mechanical power (stress power), $\dot{W}_m$ in an elastic-plastic deformation mechanism can be estimated through kinematic decomposition, Eq.(1), as

$$\dot{W}_m = \sigma \dot{F} = \sigma [\dot{U}^e R^e F^p + U^e \dot{R}^e F^p + U^e \dot{R}^e \dot{F}^p], \quad (11)$$

By using the definition of rate of plastic deformation gradient, $\dot{F}^p = \ddot{L}_p F^p$, mechanical power can be written as

$$\dot{W}_m = \sigma \left( \dot{U}^e R^e + U^e \dot{R}^e \right) F^p + \left( 1 - \sum_{i=1}^{N_t} v^i \right) \sum_{\alpha=1}^{N_s} \tau_\alpha \dot{\gamma}_\alpha + \sum_{i=1}^{N_t} \tau^i \dot{\gamma}^i. \quad (12)$$

Similarly, the rate of change of entropy due to an external thermo-mechanical load $\dot{\Pi}_m$ can be decomposed into elastic and plastic components as

$$\rho_0 \theta \dot{\Pi}_m = \rho_0 \theta \dot{\Pi}_m^e + \rho_0 \theta \dot{\Pi}_m^p. \quad (13)$$

Inelastic contribution of thermo-mechanical energy $\dot{\Pi}_m^p$ can be expressed in terms of driving potential and the corresponding flux

$$\rho_0 \theta \dot{\Pi}_m^p = \left( 1 - \sum_{i=1}^{N_t} v^i \right) \sum_{\alpha=1}^{N_s} \Phi^\alpha \dot{\gamma}_\alpha + \sum_{i=1}^{N_t} v^i \Phi^i \dot{\gamma}^i, \quad (14)$$

where $\Phi^\alpha$ and $\Phi^i$ are the thermal counterparts of resolved shear stress $\tau_\alpha$ on $\alpha$-slip system and $\tau^i$ on $i$-twin system, respectively. The parameter $\Phi^\alpha$ represents thermal contribution to slip activity of $\alpha$-slip system, hence termed as thermal slip parameter. While $\Phi^i$ denotes thermal...
contribution to twin deformation of \(i\)-twin system. It is designated as thermal twin parameter. Equation (13) can be rewritten as

\[
\rho_0 \theta \Pi_m = \rho_0 \theta \Pi_m + \left(1 - \sum_{i=1}^{N_t} \upsilon^i\right) N_s \sum_{\alpha=1}^{N_s} \Phi^\alpha \dot{\gamma}^\alpha + \sum_{i=1}^{N_t} \upsilon^i \Phi^i \dot{\gamma}^i .
\]  

(15)

The formulation of internal energy density as a result of elastic-plastic deformation of austenite includes the contributions of mechanical, thermal, and crystal defect energies. The contribution of mechanical energy is a function of elastic deformation gradient \(F^e\), while thermo-mechanical contribution is represented by the elastic part of entropy \(\Pi^e_m\). Furthermore, in order to account the effects of microstrain, which develops around or within the crystal due to interatomic defects e.g. vacancies, dislocations and voids, an additional component of energy is added in internal energy density. The energy which is needed to overcome this localized strain is termed as crystal defect energy. By considering the effects of all state variables, the functional form of internal energy per unit mass can be written as

\[
\epsilon = \hat{\epsilon}(\mathbf{F}^e, \Pi^e_m, \zeta, \upsilon, \dot{\zeta}, \dot{\upsilon}, \Pi_q) .
\]  

(16)

The differential form of Eq.(16) can be illustrated as

\[
\dot{\epsilon} = \frac{\partial \epsilon}{\partial \mathbf{F}^e} \mathbf{F}^e + \frac{\partial \epsilon}{\partial \Pi^e_m} \Pi^e_m + \frac{\partial \epsilon}{\partial \zeta} \dot{\zeta} + \frac{\partial \epsilon}{\partial \upsilon} \dot{\upsilon} + \frac{\partial \epsilon}{\partial \Pi_q} \Pi_q .
\]  

(17)

The terms in Eq. (17) sequentially refers to the rate of change of bulk strain energy, entropy due to thermo-mechanical load, crystal defect microstrain energy, twinned martensite volume fraction, and the fluxes for crystal defect energy parameter, twinned martensite volume fraction, and entropy due to heat energy. Substitution of Eqs. (12), (15), and (17) in (10) gives dissipated energy in the following form

\[
\dot{E}_d = \left(1 - \sum_{i=1}^{N_t} \upsilon^i\right) N_s \sum_{\alpha=1}^{N_s} \left(\tau^\alpha + \Phi^\alpha - \rho_0 \frac{\partial \epsilon}{\partial \zeta} \Psi^\alpha\right) \dot{\gamma}^\alpha
\]

\[
+ \sum_{i=1}^{N_t} \dot{\upsilon}^i \left(\tau^i + \Phi^i - \rho_0 \frac{\partial \epsilon}{\partial \zeta} \Psi^i\right) \dot{\gamma}^i - (\theta) \nabla \Pi_q .
\]  

(18)

where \(\upsilon^i\) is the volume fraction of \(i\)-twin system, \(N_{sl}\) and \(N_{tw}\) are the number of \(\alpha\)-slip and \(i\)-twin systems, respectively, \(\tau^\alpha\) and \(\tau^i\) are the resolved shear stress on slip and twin systems, respectively, \(\Phi^\alpha\) and \(\Phi^i\) are the thermal counterparts of resolved shear stress on slip and twin systems, respectively. \(\frac{\partial \epsilon}{\partial \zeta}\) is the partial variation of internal energy with respect to crystal defect microstrain parameter, \(\Psi^\alpha\) and \(\Psi^i\) are stress-like terms and functions of slip resistance of \(\alpha\)-slip system and twin resistance of \(i\)-twin system, respectively, and \(\Pi_q\) is the entropy flux due to heat flux \(\vec{q} (\vec{q} = \Pi_q \theta)\). The terms on the right hand side of Eq.(18) are respectively represent the slip, twin, and heat loss contributions of dissipated energy.

The Helmholtz free energy (HFE) for slip and twin based elastic-plastic deformation of a crystal can be explained using the three components of HFE i.e. mechanical \(E_{hm}\), thermal \(E_{ht}\) and crystal defect energy \(E_{hd}\). The effect of these energies in HFE becomes a function of elastic deformation gradient \(\mathbf{F}^e\), absolute temperature \(\theta\), and crystal defect microstrain parameter \(\zeta\).

\[
E_h = E_{hm} + E_{ht} + E_{hd} ,
\]  

(19)

The final form of HFE is given as
\[ E_h = \frac{1}{\rho_0} \mathbf{F}_e \mathbf{F}_p (\bar{\mathbf{C}}^{eq} : \bar{\mathbf{E}}^e \bar{\mathbf{E}}^e) (\mathbf{F}_p)^T \left[ \mathbf{F}_e + (\mathbf{F}_e)^T \right]^{-1} \]

\[ + \theta \left[ - h_{eq} \ln \left( \frac{\theta}{\theta_r} \right) + \left( h_{eq} - \Pi_{m,0}^e \right) \right] + \frac{1}{2\rho_0} \varphi G_{eq} \zeta^2 . \]

where \( h_{eq} \) is the equivalent specific heat, \( \theta_r \) is the reference temperature, \( \varphi \) is the dislocation interaction parameter, and \( G_{eq} \) is the equivalent modulus of rigidity.

The driving potentials for the plastic flow due to slip and twin mechanisms in an elastic-plastic deformation of a crystal are derived from the dissipated energy expression (Eq.(18)). Substitution of equivalent relation of HFE and the internal energy in terms of crystal defect microstrain parameter \( \frac{\partial E_h}{\partial \zeta} = \frac{\partial \epsilon}{\partial \zeta} \), and differentiation of HFE equation, Eq.(20), with respect to \( \zeta \) give the expressions for driving potentials for slip and twin plastic flow as

\[ G^\alpha = \left( 1 - \sum_{i=1}^{N_t} v^i \right) \left( \tau^\alpha + \Phi^\alpha - \rho_0 \frac{\partial E_h}{\partial \zeta} \Psi^\alpha \right) \]

\[ = \left( 1 - \sum_{i=1}^{N_t} v^i \right) \left( \tau^\alpha + \Phi^\alpha - \varphi G^\epsilon \zeta \Psi^\alpha \right) . \]

\[ \mathcal{P}^i = v^i \left( \tau^i + \Phi^i - \rho_0 \frac{\partial E_h}{\partial \zeta} \Psi^i \right) = v^i \left( \tau^i + \Phi^i - \varphi G^\epsilon \zeta \Psi^i \right) . \]

Equations (21) and (22) demonstrate that the driving potentials for slip and twin deformations vary during the course of deformation due to the dependence on resolved shear stresses \( (\tau^\alpha, \tau^i) \), thermal slip parameters \( (\Phi^\alpha, \Phi^i) \), crystal defect parameters \( (\Psi^\alpha, \Psi^i) \), and the volume fractions of untwinned \( (v^\alpha) \) and twinned \( (v^i) \) regions.

A simple power law function based on shear stress \( \tau^\alpha \) and slip resistance \( s^\alpha_r \) is used to predict the kinetics of shear flow during plastic deformation of metals (Kalidindi et al., 1992), (Marin, 2006). This power law function is given by

\[ \dot{\gamma}^\alpha = \dot{\gamma}_0 \left( \tau^\alpha \right)^{\frac{1}{m}} \sin(\tau^\alpha) , \]

where \( m \) is the strain rate sensitivity parameter and it is assumed constant in the current work. Similar to the shearing rate of \( \alpha \)-slip system, a simple power law function is used to represent the rate of change of twinned volume fraction of \( i \)-twin system \( \dot{v}^i \) as discussed in (Houtte, 1978), (Tomé et al., 1991), (Kalidindi, 1998). The rate of change of twinned volume fraction is mainly dependent on the resolved shear stress \( \tau^i \) and twin resistance \( s^i_r \) of \( i \)-twin system.

\[ \dot{v}^i = \dot{v}^i (\tau^i, s^i_r, \ldots) \]

The power law function for the rate of change of volume fraction is given as

\[ \dot{v}^i = \frac{\dot{\gamma}_0 (\tau^i)}{\gamma^i (s^i_r)^{1/m}} , \]

\[ 778 \]
The hardening of slip system is estimated through a well established PAN model (Peirce et al., 1983)

\[
\dot{s}_r^\alpha = \sum_{\beta=1}^{N_{sl}} h^{\alpha\beta} |\dot{\gamma}^\beta| ,
\]

(26)

where \( h^{\alpha\beta} \) is the latent hardening matrix, and \( \dot{\gamma}^\beta \) is the shear strain rate of \( \beta \)-slip system \( (\beta = j, j = 1, ..., i-1, i+1, ..., N_{sl}) \). The twin resistance for \( i \)-twin system in the current hardening model is used as proposed by (Kalidindi, 2001)

\[
\dot{s}_t^i = h_{nc}^i \left( \sum_{i=1}^{N_{tw}} u^i \right)^d \sum_{\mu_1=0}^{\gamma^i} \dot{\gamma}^\mu_1 + h_{cp}^i \left( \sum_{i=1}^{N_{tw}} u^i \right) \sum_{\mu_2=0}^{\gamma^i} \dot{\gamma}^\mu_2,
\]

(27)

where \( h_{nc}^i \) and \( h_{cp}^i \) are the initial hardening rates for non-coplanar and co-planar twin systems \( i \) to \( \alpha \)-slip system, respectively, \( \sum_{i=1}^{N_{tw}} u^i \) represents the total volume of \( i \)-twin systems, \( d \) is a material parameter, \( \mu_1 (\mu_1 \in i) \) represents the number of non-coplanar twin systems, \( \gamma^i \) is the shear strain of \( i \)-twin system, \( \dot{\gamma}^\mu_1 \) is the rate of change of volume fraction of non-coplanar twin systems, \( \mu_2 (\mu_2 \in i) \) is the number of co-planar twin systems, and \( \dot{\gamma}^\mu_2 \) is the rate of change of volume fraction of co-planar twin systems to twin system \( i \). The first term on the right hand side of Eq. (27) shows the twin hardening due to the formation of non-coplanar twins, while the second term represents the contribution to twin hardening due to an evolution of co-planar twins.

**NUMERICAL MODELING**

Numerical computations are carried out for single and polycrystal FCC-austenite using the commercial finite element analysis software ABAQUS with user-defined subroutines to incorporate the constitutive model developed in this work. A single crystal is modeled as one 8-node brick finite element of unit side lengths with reduced integration (C3D8R one point integration). For polycrystalline simulations, each finite element represents 500 grains of random crystallographic texture. The developed numerical model is validated through the published literature and then finite element simulations are performed for combined loading condition, as shown in Figure 2. The combined loading focussed on uniaxial tension with shear. This replicates the complex loading condition which exists in material forming processes like pipe expansion, extrusion, rolling, etc. The effects of texture on elastic-plastic deformation are considered by performing the simulations for three different crystallographic orientations i.e. [100], [110], and [111].

Material parameters include elasticity tensor elements of austenite as reported in (Turkeltaub and Suiker, 2006). These include: \( C_{11}^a = 286.6 \), \( C_{12}^a = 166.4 \), and \( C_{44}^a = 145.0 \) in GPa. The elasticity tensor elements are obtained using heuristic approach through the analysis of nano-indentation experiments performed on a TRIP steel with 0.92 wt% of austenite phase (Furnemont et al., 2002). Other material parameters include modulus of rigidity \( G^a \) and bulk modulus \( K^a \) which are calculated using isotropic relations defined for cubic crystals as: \( G^a = \frac{1}{3}(C_{11}^a - C_{12}^a + 3C_{44}^a) \), and \( K^a = \frac{1}{3}(C_{11}^a + 2C_{12}^a) \). This gives \( G^a = 111.0 \) GPa and \( K^a = 206.5 \) GPa. The density of austenite is taken as of carbon steel i.e. \( \rho_0 = 7.8x10^{-6} \) kg/mm\(^3\). The hardening parameters include: initial hardening rate (assumed to be identical for all \( \alpha \)-slip systems) \( h_{0}^\alpha = 350 \) MPa, initial slip resistance \( s_{r,0}^\alpha = 80 \) MPa, initial saturation value of slip resistance \( s_{r,s0}^\alpha = 380 \) MPa, saturation slip resistance exponent \( a = 0.005 \), and shear strain rate
Figure 2: Finite element model with specified tension-shear boundary condition

at saturation slip resistance $\dot{\gamma}_{S_0} = 5 \times 10^{10} \text{ s}^{-1}$. In the present model, the latent hardening coefficient for slip-slip and slip-twin interactions is taken identical as $q^{\alpha\beta} = 1.4$. The other slip and twin hardening parameters are estimated as: material slip hardening parameter $s_{r,p} = 350$ MPa, material parameter $d = 0.05$, initial hardening rates for non-coplanar and co-planar twin systems are respectively, $h^{i}_{nc} = 800$ MPa and $h^{i}_{cp} = 8000$ MPa. The values of these two parameters are based on an assumption that the co-planar twin systems contribute more than non-coplanar in the hardening of an austenite crystal. In addition, the kinetic flow parameters include initial value of shear strain rate of $\alpha$-slip system $\dot{\gamma}_0$ and rate sensitivity parameter $m$. These two parameters are selected in such a manner that the overall deformation response becomes nearly rate-independent. The values of kinetic flow parameters are taken as $\dot{\gamma}_0 = 0.001 \text{ s}^{-1}$, and $m = 0.02$.

RESULTS AND DISCUSSION

Model Validation

In order to validate the developed slip and twin based crystal plasticity model, finite element simulations are performed for polycrystal brass subjected to simple compression. The simple compression experiment was performed by (El-Danaf et al., 2001) on annealed 70/30 brass, which is classified as low stacking fault energy alloy. The test was performed at an equivalent strain rate of 0.001 - 0.0015 $\text{ s}^{-1}$. The displacement of -0.35 mm is applied in $e^1_3$ axis on a surface having area normal parallel to $e^1_3$ direction. The annealed brass is assumed to consists of random but isotropic initial texture of 500 grains. The orientation distribution function (ODF) of these grains are defined in terms of Euler angles based on Kocks convention. The material parameters (elasticity tensor elements) are taken as: $C^{\alpha}_{11} = 183.7$, $C^{\alpha}_{12} = 90.5$, and $C^{\alpha}_{44} = 46.6$ in GPa. The hardening parameters include: initial slip hardening rate $h^0_{\alpha} = 200$ MPa, initial slip resistance $s^0_{r,\alpha} = 21$ MPa, initial saturation value of slip resistance $s^0_{r,S_0} = 120$ MPa, saturation slip resistance exponent $a = 0.001$, and shear strain rate at saturation slip resistance $\dot{\gamma}_{S_0} = 5 \times 10^{10} \text{ s}^{-1}$. The latent hardening coefficient is $q^{\alpha\beta} = 1.4$. The values of kinetic flow parameters are taken as $\dot{\gamma}_0 = 0.001 \text{ s}^{-1}$, and $m = 0.02$. The initial value of twin resistance is $s^i_{t,0} = 60$ MPa. Other twin hardening parameters are estimated as: material slip hardening parameter $s_{r,p} = 350$ MPa, material parameter $d = 0.05$, initial hardening rates for non-coplanar and co-planar twin systems are respectively, $h^{i}_{nc} = 500$ MPa and $h^{i}_{cp} = 8000$ MPa.

Figure 3 shows the comparison of experimental and finite element simulation equivalent stress-strain behavior in simple compression using the material and hardening parameters as described above. Although, the simulation model overestimates (maximum of 56 MPa) in
Figure 3: Experimental and simulation stress-strain response of 70/30 brass in simple compression between 0.1 to 0.3 equivalent strain and underestimates (maximum of 68 MPa) at higher strain, it is in general good agreement with the experimental result.

Using similar modeling parameters, the material is subjected to load depicting simple shear. Figure 4 shows the comparison between experimental and simulation results. It can be observed that the simulation model compares well with experiment. The model is overestimating the measured results at higher strains (≥ 0.2). This is due to the higher value of saturation slip resistance due to slip-slip and slip-twin interactions. These interactions may lead to the higher hardening. It can also effects the experimental results but the presence of grain to grain
interaction, dislocation interactions, presence of voids, etc. in the material may result in higher or lower values of stress. These interactions are not present in the simulation result. In both cases, the simulation results agrees well with experimental observations with an acceptable error of ± 10%.

**Combined Loading: Tension-Shear**

In many applications of metal forming processes, complex loading conditions (combination of tension, compression, shear etc.) can exist. In order to replicate these real cases, a combined load of tension and shear is applied on a single and polycrystal of austenite. In this section, the stress-strain response, variation of Cauchy stress components, magnitude of shear strain, and volume fraction of twinned martensite of single and polycrystal austenite subjected to tension-shear are discussed.

![Graph showing the variation of equivalent stress versus equivalent strain for single and polycrystal austenite under combined load of tension and shear](image)

**Figure 5:** Equivalent stress versus equivalent strain for single and polycrystal austenite under combined load of tension and shear

The variation of equivalent stress-strain for single and polycrystal austenite are shown in Figure 5. It is obvious that austenite single crystal loaded in [111] direction exhibits highest magnitude of equivalent stress, while crystal loaded in [100] and [110] directions experience much lower and almost identical stresses. Polycrystal austenite shows similar behavior but intermediate values of equivalent stress at low values of equivalent strain (< 0.3). However, a strain softening phenomenon is observed in polycrystal austenite near equivalent strain of 0.3 and then re-hardening occurs for equivalent strain greater than 0.35. This fluctuating behavior of polycrystal austenite (hardening - softening - higher hardening) shows that at high strain levels the interaction between slip and twin systems becomes more active and thus more energy is required for the plastic flow. As mentioned before that softening may occur due to the re-orientation of grains. In addition, in twin based elastic-plastic deformation, softening may also occur due to the activation of twin planes, which dissipates energy and reduce the overall stress of the material. The convergence issues are observed in the simulations once material experiences softening (due to the negative stiffness matrix) especially in complex loading conditions. These convergence issues are resolved by reducing the time step size until the convergence of
solution. This technique is actually a trade off between convergence and computational time. In future, other convergence techniques could also be used like line search algorithm. Although crystallographic directions [100] and [110] show identical stress-strain behavior, a significant difference is observed in their yield stresses (for [100] and [110] directions 192 MPa and 230 MPa), respectively. An austenite crystal loaded in [111] direction exhibits highest value of yield stress (302 MPa), while polycrystal austenite yields at 217 MPa.

![Variation of cumulative shear strain induced by active slip and twin systems subjected to combined tension and shear](image)

Variation of cumulative shear strain for slip and twin based elastic-plastic deformation of single crystal austenite is shown in Figure 6. Shear strain due to slip activity is shown by dotted lines, while shear strain due to twin deformation is shown by symbols. It is evident that for [100] and [110] directions the contribution of slip is significantly higher than twin. While in [111] direction, both modes show similar contribution to plastic deformation. The difference in contribution show that the activity of slip and twin systems as well as their interactions are dependent on the loading direction.

The variation in the twin volume fraction with respect to equivalent strain for a single crystal austenite loaded in three directions is shown in Figure 7. It is clear that the variation of volume fraction of twinned martensite behaves nonlinearly for [100] and [111] directions, while linear for [110] direction. As discussed previously, the nonlinearity in the variation of volume fraction might be due to the interactions among slip and twin systems. A substantial increase in the volume fraction for [100] direction at higher strain (> 0.3) may be because of the activation of number of twin systems due to an increase in the driving potential and/or reduction in the slip-twin and twin-twin interactions. The nonlinear variation in twin volume fraction is observed for [100] and [111] directions. This is possibly due to the hardening of crystal due to slip-slip and slip-twin interaction which affects the twin volume fraction rate.

**CONCLUSIONS**

Twin based crystal plasticity model is developed in order to predict twinning induced plasticity behavior in austenitic steels. A stress-strain constitutive relation is developed through the
kinematic decomposition of deformation into intermediate configurations. A thermodynamic framework is used to formulate driving potential, dissipated and Helmholtz free energy. The plastic flow and hardening rules for slip and twin mechanisms are formulated with the consideration of slip-twin and twin-twin interactions. Finite element simulations are done for combined load of tension and shear. In combined tension-shear load, strain softening and re-hardening phenomena are observed in polycrystal austenite. The alternating (hardening - softening - higher hardening) behavior is expected due to the variation in the interaction among slip and twin systems. Slip mechanism is found the dominant mode of plastic deformation in [100] and [110] direction, while both slip and twin modes contribute same for [111]. The nonlinear variation in [100] and [110] directions is possibly due to the slip-slip and/or slip-twin interactions. The observations and analysis of results are expected to provide a meaningful understanding about the behavior of TWIP steels under thermo-mechanical load.

References

Allain, S., Chateau, J. P., and Bouaziz, O. (2004). A physical model of the twinning-induced plasticity effect in a high manganese austenitic steel. *Materials Science and Engineering: A*, 387-389:143–147.

Asgari, S., El-Danaf, E., Kalidindi, S. R., and Doherty, R. D. (1997). Strain hardening regimes and microstructural evolution during large strain compression of low stacking fault energy fcc alloys that form deformation twins. *Metallurgical and Materials Transactions A*, 28(9):1781–1795.

Bhattacharyya, K. (1991). Wedge-like microstructure in martensites. *Acta Metallurgica et Materialia*, 39(10):2431–2444.

Bouaziz, O. (2012). Strain-hardening of twinning-induced plasticity steels. *Scripta Materialia*, 66(12):982–985.
Bouaziz, O., Allain, S., Scott, C. P., Cugy, P., and Barbier, D. (2011). High manganese austenitic twinning induced plasticity steels: A review of the microstructure properties relationships. Current Opinion in Solid State and Materials Science, 15(4):141–168.

El-Danaf, E., Kalidindi, S. R., and Doherty, R. D. (2001). Influence of deformation path on the strain hardening behavior and microstructure evolution in low SFE FCC metals. International Journal of Plasticity, 17(9):1245–1265.

Furnémont, Q., Kempf, M., Jacques, P. J., Göken, M., and Delannay, F. (2002). On the measurement of the nanohardness of the constitutive phases of TRIP-assisted multiphase steels. Materials Science and Engineering: A, 328(1-2):26–32.

Houtte, P. V. (1978). Simulation of the rolling and shear texture of brass by the Taylor theory adapted for mechanical twinning. Acta Metallurgica, 26:591–604.

Kalidindi, S. R. (1998). Incorporation of deformation twinning in crystal plasticity models. Journal of the Mechanics and Physics of Solids, 46(2):267–290.

Kalidindi, S. R. (2001). Modeling anisotropic strain hardening and deformation textures in low stacking fault energy fcc metals. International Journal of Plasticity, 17(6):837–860.

Kalidindi, S. R., Bronkhorst, C. A., and Anand, L. (1992). Crystallographic texture evolution in bulk deformation processing of fcc metals. Journal of the Mechanics and Physics of Solids, 40(3):537–569.

Khosravani, A., Scott, J., Miles, M. P., Fullwood, D., Adams, B. L., and Mishra, R. K. (2013). Twinning in magnesium alloy AZ31B under different strain paths at moderately elevated temperatures. International Journal of Plasticity, 45:160–173.

Lee, E. H. (1969). Elastic-plastic deformation at finite strains. Journal of Applied Mechanics, 36(1):1–6.

Marin, E. B. (2006). On the formulation of a crystal plasticity model. Technical report, Sandia National Laboratories, New Mexico and Livermore.

Peirce, D., Asaro, R. J., and Needleman, A. (1983). Material rate dependence and localized deformation in crystalline solids. Acta Metallurgica, 31(12):1951–1976.

Peng, X., Zhu, D., Hu, Z., Yi, W., Liu, H., and Wang, M. (2013). Stacking fault energy and tensile deformation behavior of high-carbon twinning-induced plasticity steels: Effect of Cu addition. Materials & Design, 45:518–523.

Shiekhsouk, M. N., Favier, V., Inal, K., and Cherkaoui, M. (2009). Modelling the behaviour of polycrystalline austenitic steel with twinning-induced plasticity effect. International Journal of Plasticity, 25(1):105–133.

Tamarelli, C. M. (2011). The evolving use of advanced high strength steels for automotive applications. Technical report, University of Michigan, USA, Materials Science and Engineering Department.

Tomé, C. N., Lebensohn, R. A., and Kocks, U. F. (1991). A model for texture development dominated by deformation twinning: Application to zirconium alloys. Acta Metallurgica et Materialia, 39:2667–2680.
Turteltaub, S. and Suiker, A. S. J. (2006). A multiscale thermomechanical model for cubic to
tetragonal martensitic phase transformations. *International Journal of Solids and Structures*,
43(14-15):4509–4545.

Wang, J. and Sehitoglu, H. (2013). Twinning stress in shape memory alloys: Theory and
experiments. *Acta Materialia*, 61(18):6790–6801.