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On the feasibility of partial slip reversal and de-twinning during the cyclic loading of TWIP steel

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ABSTRACT

A recently modified Elasto-Plastic Self-Consistent (EPSC) model which empirically accounts for both *intergranular* and *intragranular* back stresses has been successfully used to simulate the cyclic (tension-compression) loading behaviour of an Fe-24Mn-3Al-2Si-1Ni-0.06C TWinning Induced Plasticity (TWIP) steel between strain limits of $\pm 1\%$. Lattice strain measurements acquired via in-situ neutron diffraction were used to further validate the modelling results. An improved prediction of the pronounced Bauschinger effect during unloading is achieved when the reversibility of partial slip in the $\langle 112 \rangle$ direction is accounted for. This result indicates a potential contribution of the stress-induced separation of partial dislocations to the observed early yielding at the low strain levels employed in this study. It also raises the possibility that de-twinning events could be operative during load reversal.

1. Introduction

TWinning Induced Plasticity (TWIP) steels comprise a stable face-centred cubic (fcc) austenite phase with low stacking fault energy (SFE = 18–40 mJ/m^2) that promotes deformation accommodation via twinning along with dislocation glide. This low SFE also facilitates the dissociation of perfect dislocations gliding on the $\{111\}$ plane in the $\langle 110 \rangle$ direction into $\langle 112 \rangle$ Shockley partials ($a/2[10\bar{1}] \rightarrow a/6[11\bar{2}] + a/6[2\bar{1}\bar{1}]$) bounding stacking faults.

While the modelling of the *monotonic* deformation behaviour of TWIP steel has been the focus of numerous studies (see [1,2] and the references therein), the modelling of its cyclic (reverse) loading remains very limited. In this regard, we recently applied a combination of in-situ neutron diffraction and a modified Elasto-Plastic Self-Consistent (EPSC) modelling scheme to a TWIP steel subjected to cyclic (tension-compression) loading [3]. A pronounced Bauschinger effect was observed upon load reversal (or early yielding during unloading) and was attributed to a combination of *intergranular* residual stresses and *intragranular* sources of back stress such as dislocation pile-ups at the intersection of stacking faults. The modified EPSC model has been successfully used to simulate the macroscopic stress-strain response and the evolution of the lattice strains.

While our simulations in [3] considered both perfect slip and twinning (via the “twinning scheme” of Clausen et al. [4]), the potential contribution of partial slip to the overall mechanical response was not taken into account. The present study is therefore the first to assess the influence of deformation faulting or slip by partials during the cyclic loading of a TWIP steel, such that we provide a more holistic analysis of the contribution of perfect/partial slip and twinning to the overall deformation behaviour. The implications of slip reversal along the $\langle 112 \rangle$ direction before and after the initiation of twinning are also discussed.

2. Material and methods

A cast slab of a Fe-24Mn-3Al-2Si-1Ni-0.06C wt% TWIP steel was 52% hot rolled, 42% cold rolled and then annealed at 850 °C for 300 s to obtain a fully recrystallised microstructure. A round tension/compression sample of 7.62 mm gage length and 2.54 mm diameter was machined with its gage length parallel to the rolling direction. In-situ neutron diffraction measurements during cyclic tension-compression loading between strain limits of $\pm 1\%$ were performed on the SMARTS diffractometer at Los Alamos Neutron Science Center. Five complete tension-compression cycles were performed followed by a sixth tension half cycle. The changes in the individual peak positions were used to calculate the $\{hkl\}$

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specific lattice strains by $\varepsilon_{hkl} = (d_{hkl} - d^0_{hkl})/d^0_{hkl}$, where, d_{hkl} and d^0_{hkl} are the instantaneous and unstrained lattice spacing, respectively. Further experimental and analytical details are given in [3].

3. Elasto-plastic self-consistent modelling

In the EPSC model [5], the elastic response of the individual grains is described by the single crystal elastic constants (C_{11}=161.5 GPa, C_{12}=110.3 GPa and C_{44}=133.3 GPa) [3], whereas the plastic response is described by activating the various deformation systems (s) at predetermined values of the critical resolved shear stress (CRSS). The CRSS evolves with the total accumulated shear strain ($\Gamma = \sum_s \Delta\gamma^s$) following an extended Voce hardening rule:

$$\tau^s_{for} = \tau^s_0 + \left(\tau^s_{1,for} + \theta^s_{1,for}\Gamma\right)\left[1 - \exp\left(-\frac{\theta^s_{0,for}\Gamma}{\tau^s_{1,for}}\right)\right] \tag{1}$$

Here τ^s_{for} represents the *isotropic* hardening associated with the non-directional accumulation of obstacles such as forest dislocations and/or deformation twin boundaries. Since the EPSC model allows for variations in stress and strain between different grains (orientations), it can inherently capture the effect of the *intergranular* stress but not the *intragranular* stress. Consequently, the model was recently modified[1] to include a back stress term (τ^s_{bs}) in order to account for the *kinematic* hardening in individual slip systems as it reduces the resolved applied stress by the directional back stress arising from the pile-up of dislocations at various barriers [6]:

$$\tau^s_{bs} = \left[\left(\tau^s_{1,bs} + x^s_0\right) + \theta^s_{1,bs}\left(\gamma^s - \gamma^s_0\right)\right]\left[1 - \exp\left(-\frac{\theta^s_{0,bs}\left(\gamma^s - \gamma^s_0\right)}{\left(\tau^s_{1,bs} + x^s_0\right)}\right)\right] \tag{2}$$

In (Eqs. (1) and 2), τ^s_0 and τ^s_1 are the initial and back extrapolated CRSS and θ^s_0 and θ^s_1 are the initial and final asymptotic hardening rates for the forest hardening (*for* in Eq. (1)) and back stress (*bs* in Eq. (2)) formulations. The γ^s_0 and x^s_0 terms are the strain and stress "memory" parameters which are both initially set to zero during the first forward half cycle. Please refer to [3–6] for further details on the EPSC model.

The initial texture input for all simulations comprised 5000 discrete orientations calculated from the fully annealed texture. Two modelling cases[2] have been applied as follows:

(1) Case I utilises the twinning scheme of Clausen et al. [4] which was applied in [3], and included here for comparison with Case II. This scheme accounts for the stress relaxation associated with twin formation via the so called "finite initial fraction" approach; wherein the twin is assumed to grow to a fixed volume fraction of its parent grain at the nucleation stage. Here the plastic shear of the twinning system generates a back stress between the parent and the twin due to the constraint of the surrounding polycrystalline aggregate.
In Case I, 24 {111}⟨110⟩ perfect slip systems (counting both forward and reverse slip directions) and 12 {111}⟨112⟩ forward twinning systems (due to the unidirectional nature of twinning) were introduced into the EPSC model.

(2) Case II assesses the contribution of deformation faulting or slip by partials and is based on the idea suggested by Hu et al. [7] to explain the transition from Copper to Brass–type textures in low SFE fcc materials. The original mechanism involves glide on a fixed {111} slip plane in either the conventional ⟨110⟩ or partial ⟨112⟩ directions. In other words, the {111}⟨112⟩ systems do not contribute to deformation accommodation as twinning systems, but as partial slip systems with reversible glide along the ⟨112⟩ direction. Perfect slip was also suppressed in Case II, such that only 24 {111}⟨112⟩ partial slip systems (counting both forward and reverse slip directions) were considered, in order to isolate the effect of deformation faulting from perfect slip. A similar approach was adopted previously by Saleh et al. [1] and Beyerlein et al. [8] during the Visco-Plastic Self-Consistent modelling of monotonic tensile loading (TWIP steel) and rolling (Ag-Cu cast eutectic nanocomposite) textures in low SFE fcc materials.

It is emphasised that while the above two modelling cases assess different aspects of TWIP steel deformation behaviour, the physical reality of deformation accommodation is the result of the concurrent and competing interaction between perfect/partial slip and twinning.

4. Results and discussion

The Voce hardening parameters (Table 1) were adjusted until optimal agreement with the macroscopic stress-strain was achieved for Cases I and II (Fig. 1). In Fig. 1a only Case II is shown for brevity. The experimental hysteresis loop is generally well captured such that the simulated macroscopic flow stress tends to saturate with further cycling and it closely follows the gradual elasto-plastic transition upon load reversal. As seen in Fig. 2 (and similar to Case I predictions in Figure 7, Ref. [3]), Case II also returns good agreement with the lattice strains such that the shape, magnitude and width of the lattice strain hysteresis loops of the {111}, {200} and {220} grain families are reasonably predicted.

The adequacy of Cases I and II in describing the underlying deformation mechanisms is assessed via two experimental features: (i) the Bauschinger effect or early yielding during unloading (Fig. 1b) and (ii) the tension-compression asymmetry (Fig. 1c).

With respect to the early yielding and the associated elasto-plastic transition upon load reversal (Fig. 1b), it is seen that Case I provides reasonable agreement with the experimental macroscopic stress-strain curve as it accounts for the stress relaxation effect incorporated in the twinning scheme; such that back stress is enforced between the parent and the twin upon the creation of the latter. However the partial slip approach of Case II follows the macroscopic stress-strain curve even more closely than Case I during unloading as it mimics the early reverse yielding of the experimental data.

Prior to twin formation, i.e., before the divergence of the dissociated partial dislocations to an infinite separation distance with increasing stress [9], the improved agreement of Case II is in accordance with the stress-induced separation of partial dislocations idea; as slip on the {111}⟨112⟩ systems is allowed to change direction during load reversal. It is argued that while partial dislocations are pulled apart during forward loading, they tend to restore their equilibrium separation distance upon unloading [10]. In turn, both the associated stored energy release and the change in slip direction during load reversal can provide additional sources of back stress in low SFE materials.

Following the initiation of twinning, the improved prediction of Case II raises the possibility that de-twinning events associated with the reversibility of slip along the ⟨112⟩ direction could also be occurring. To the best of our knowledge, no unambiguous observation of de-twinning has been made during reverse loading of

[1] Please note that the modified EPSC model strictly deals with load reversal at small strains; where the Bauschinger effect is mostly related to the reversal of dislocation motion.

[2] In both cases, equal latent hardening is imposed such that all deformation systems are assumed to contribute equally to the hardening of each other.