Full-Field Crystal Plasticity Modeling of $\{10\bar{1}2\}$ Twin Nucleation

YubRaj Paudel, Christopher D. Barrett, and Haitham El Kadiri

Abstract

Historically, the ability of crystal plasticity to incorporate the Schmid's law at each integration point has been a powerful tool to simulate and predict slip-induced localization at the single and polycrystal levels. Unfortunately, this remarkable capability has not been replicated for materials where twinning becomes a noticeable deformation mechanism. The challenge resides mainly in the biased regional lattice transformation associated with twin formation in defiance of its obedience to threshold stress. Inspired by results from micromechanics, digital image correlation, and molecular dynamics, we developed an explicit twinning nucleation criterion based on hydrostatic stress gradient and volume fraction of twin inside a grain. Characteristic twin spacing parameter is used as a function of twin height to determine site-specific nucleation points in the case of multiple twins. This approach offered a good reproduction of the microstructure evolution and autocatalysis phenomenon as affected by twinning in a tricrystal system.

Keywords

Crystal plasticity • Hydrostatic stress • Twin spacing

Introduction

Twinning is referred to as a "double edged sword" mechanism because of its ability to increase strength and ductility in a low-stacking fault energy cubic crystal system, however, it reduced ductility, anisotropy, and damage in orthorhombic and hexagonal close-packed (hcp) structures. In hcp metals, the lack of "easy" slip modes to accommodate $\langle c \rangle$-axis tension/compression [1] at low temperatures/high strain rates stokes a whole host of shear localization phenomena, including twinning and pyramidal $\langle c + a \rangle$ slip. Twinning is a particular challenge as its polarity and lattice reorientation tend to cause strong asymmetry and anisotropy, respectively, which increases with texture strength. Furthermore, it has been shown that twinning interaction with microstructural defects contributes to strain incompatibilities and damage initiation [2].

In recent years, experimental studies through scanning electron microscope (SEM) and transmission electron microscope (TEM) along with atomistic simulations have shown several mechanisms associated with twinning such as twin–twin interaction [3–6], slip–twin interaction [7, 8], detwinning [9–11], twin–grain boundary interactions [12–14], and double twinning [15, 16]. At the microscale level, substantial efforts have been made to understand the mechanisms associated with twin nucleation, propagation, and growth, and upscale them to crystal plasticity models [17–22].

Crystal plasticity techniques have been a powerful tool to simulate and predict the slip behavior at the grain level and the subsequent heterogeneous stress/strain localization and texture evolution at the macroscopic level. In hexagonal close-packed (hcp) metals, crystal plasticity based on finite element methods (CPFEM) [11, 20, 23–26] and fast-Fourier transform (CPFFT) [21, 22, 27, 28] has been employed to capture the heterogeneous deformation behavior of twinning. However, most of the models lag physically motivated twin incorporation that reflects the early stages of embryonic

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J. B. Jordon et al. (eds.), *Magnesium Technology 2020*, The Minerals, Metals & Materials Series, https://doi.org/10.1007/978-3-030-36647-6_23

twin nucleation and lengthwise burst. Most of the full-field crystal plasticity models employ phenomenological criteria to capture twinning, exemplified by pseudo-slip approach, absence of site-specific twin nucleation, and ensuing lack of reproducing the observed twin spacing including the case of multivariant twinning. Likewise, the evolution of deformation twins with strain, and ultimately calculations of constitutive response along with proper description of twin interfaces and twin boundaries are yet to be incorporated in crystal plasticity models. The Schmid factor based on far-field stress is inadequate to describe variant selection [29] and dynamics of twin expansion. The dependence of the twin nucleation stress on the grain size [30] has not yet been quantified in crystal plasticity models. In recent years, some of the full-field crystal plasticity approaches have been successful to introduce a site-specific twin nucleation [26, 31]; however, they do not ratify all the features of twinning and twin interfaces.

For any compound twin, a recent theory provides an analytical solution for the vector displacements for both shear and shuffle [32]. Shear, which is the most fundamental and unquestionable condition for dislocation and disconnection motion, is associated with the Schmid behavior. However, shuffles are related to the atomic movement due to diffusion. In general, the only component of stress that drives diffusion is the hydrostatic pressure or more precisely gradient of hydrostatic pressure. As shuffle is a pure diffusion phenomenon, it could be readily sensitive to the local state of hydrostatic pressure in the disconnection core as its glide along the twin interface. In an experimental study [33], an inherent difference in the stress state between contraction and compression showed profound implications on the ease of shuffle and the mobility of disconnections. A complex stress state acting on the $\langle c \rangle$-axis of the unit crystal lattice aided the shuffle associated with twin formation thereby reducing the required stress to induce shear through twinning or slip [33]. Inspired by these results stressing the effect of shuffles on twin nucleation and disconnection core width, we developed an explicit twinning nucleation criterion based on hydrostatic stress gradient and volume fraction of twin inside a grain.

Twinning-Induced Microstructure

Proust et al. [34] showed that profuse twinning followed by rapid strain hardening led to a strain–path anisotropy in highly textured Mg alloy. Studies have shown that the high strain hardening is caused due to interactions between the twinning-induced microstructure and slip activities [3, 8, 17, 35, 36]. The dislocation transmutation reactions and slip–twin interactions are clearly evident through abundantly available residual slips in the vicinity of twin boundaries as

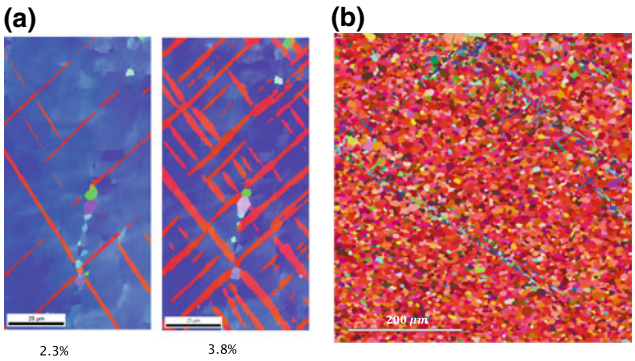

Fig. 1 **a** Twinning-induced microstructure inside a single grain in Mg AM30 specimen [3] and **b** Twinning patterns in a polycrystal Mg AZ31 specimen during three-point bending [40]

observed from the TEM experiments [37]. A twinning-induced microstructure within a single grain of extruded Mg AM30 specimen under compression is also shown in Fig. 1a [3]. In a twinning-induced microstructure, a vivid characteristic twin spacing can be observed during twinning that should be quantified and upscaled to the crystal plasticity models. These characteristic twin spacings that depend on the height of twins [38] are observed in polycrystal with strongly basal texture [39, 40].

In Mg polycrystal, a characteristic twin spacing parameter was observed during three-point bending of strongly basal textured Mg AZ31 alloy [38]. As seen in Fig. 1b, a localized twinning pattern was observed with twins across multiple grains because of autocatalysis. Autocatalysis of a twin at low-angle misorientation boundary has previously been observed in many studies [40–42]. A micromechanical solution for an ellipsoidal twin in an infinite-half space domain showed that this characteristic twin spacing can be determined through the study of elastic response of a twin and it is directly proportional to the height of twin [38]. A digital image correlation (DIC) analysis performed on three-point bending of Mg AZ31 showed that the twinning-induced microstructure evolution follows the same characteristic twin spacing behavior predicted by a micromechanical-based analytical solution [40].

New Crystal Plasticity Approach

As shuffles play an important role in atomic movement during disconnection glide, we justifiably added the contribution of hydrostatic stress gradient contribution to twin nucleation stresses as they pertain to diffusion which excludes contribution from deviatoric stresses. This initiative is well supported by various experimental findings and atomistic simulations emphasizing the role of defects in twin nucleation and mode selection. We naturally used a volume

fraction to determine twinning nucleation and used characteristic twin spacing that is a function of twin height to determine twinning-induced microstructure evolution.

In the current work, we will focus on crystal plasticity fast-Fourier transform (CPFFT) to incorporate the explicit twinning to accommodate deformation [43]. The elastic response for the twin is obtained using the technique used by Kumar et al. [21]. After each deformation step, strain and stress fields are determined based on the Green's function method solved using Lagrangian–Newton–Raphson method. The shear rate at each slip and twin systems is ensured by Eq. 1 at each integration point.

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha}\left|\frac{\tau^{\alpha}}{g^{\alpha}}\right|^{\frac{1}{m}} \tag{1}$$

The twinning criterion is based on the hydrostatic stress across the representative volume element (RVE) to determine whether twin forms or not within a grain. Twinning is the localized event and twin nucleation process is influenced by both shear and shuffle. In most of the twinning criteria, only the shear portion of twin is considered to determine whether the twin nucleated or not. However, shuffle is an important mechanism that ensures twinning through a diffusion process. Since diffusion is a function of hydrostatic pressure, the hydrostatic stress field in the material domain should be used as a twinning criterion. The hydrostatic stress (σ_h) at any integration point can be determined by:

$$\sigma_h(x) = \frac{1}{3}\sum_i \sigma_{ii}(x) \tag{2}$$

The gradient of hydrostatic stress can then be calculated by

$$\nabla_i \sigma_h(x) = \frac{\sigma_h(x+x_i) - \sigma_h(x)}{\delta x_i} \tag{3}$$

Based on the accumulated twinning shear at each point, the twin volume fraction (f) at each integration point in a RVE is determined using Schmid's law.

$$f(x) = \sum^{t} \dot{f}(x)\Delta t = \sum^{t} \frac{\dot{\gamma}(x)}{\gamma_{\text{tw}}}\Delta t \tag{4}$$

The volume fraction for twin systems in each grain is then calculated as the sum average of volume fraction at each point inside of the grain, i.

$$f^{\alpha}_{\text{grain}^i} = \frac{V(x)}{V(\text{grain}^i)}\sum_{x}^{\text{grain}^i} f^{\alpha}(x) \tag{5}$$

where $V(x)$ is the volume of each integration point and $V(\text{grain}^i)$ is the volume of each grain.

The twinning is nucleated with either of the two conditions:

1. if the gradient of hydrostatic pressure reaches a threshold value and/or
2. if the volume fraction of the grain reaches a threshold volume fraction.

The first condition allows for a twin to nucleate at the requirement of strain triaxiality. This addresses the issue of autocatalysis as the strain accommodated by a twin at a grain boundary creates stress triaxiality, when the gradient is enough, new twin nucleates. In the second case scenario, if the volume fraction within a grain is greater than the threshold volume fraction for that twin variant, then the twin nucleates. However, the number of twins nucleated depends upon the twin variant, grain morphology, and grain size. When nucleating a twin, a minimum thickness of twin is assumed. Based on the volume fraction of twin, the number of twin is determined by:

$$N^{\alpha}_{\text{twins}}(\text{grain}^i) = \frac{f^{\alpha}(\text{grain}^i)V(\text{grain}^i)}{t_{\text{tw}} * A^{\alpha}_{\text{tw}}(x_0)} \tag{6}$$

where $f^{\alpha}(\text{grain}^i)$ is the volume fraction of twin system α, $V(\text{grain}^i)$ is the volume of grain, t_{tw} is the minimum twin thickness, and $A^{\alpha}_{\text{tw}}(x_0)$ is the area of the twinning plane inside a grain. x_0 is the position of maximum gradient of hydrostatic pressure inside of the grain.

During nucleation of multiple twins at a time, a characteristic twin spacing parameter, k, is used to determine the separation distance between the twins. Twinning spacing, which is a function of twin height, is defined by:

$$h_{\text{tw}} = k \times \sqrt{A_{\text{tw}}} \tag{7}$$

where A_{tw} is the area of the twinning plane in the grain used to calculate length of the twin.

The viscoplastic FFT formulation, modified to account for site-specific twin nucleation and characteristic twin spacing, is applied to predict the local behavior of tricrystal unit cells. The stress–strain response shows drops in von-Mises stress that corresponds with the formation of twins, which reflect the plateau in stress–strain curve during profuse twin nucleation. The site-specific twin is inserted for only predominant twin variant resulting single twin variant nucleated at every grain. However, this approach can be used to ensure multiple twin variants in a single twin.

Figure 2a shows the (1 $\bar{1}$ 0 2)[$\bar{1}$ 1 0 1] twin variant nucleation in grain 2 at strain 0.7%. The lower twin in grain 2 nucleates at the tip of the twin in grain 1, whereas other two twins in grain 2 follow characteristic twin spacing to nucleate. The von-Mises stress in Fig. 2b shows the stress field as a

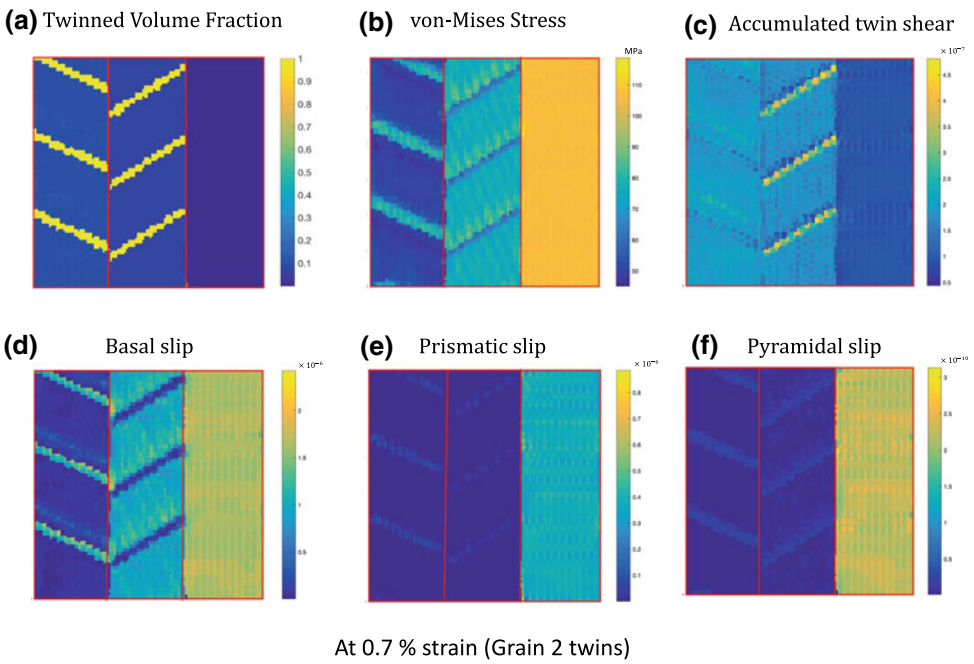

Fig. 2 At 0.7% strain, **a** (0 $\bar{1}$ 1 2) [0 1 $\bar{1}$ 1] twin variant nucleates at grain 1 and (1 $\bar{1}$ 0 2)[$\bar{1}$ 1 0 1] twin variant nucleates at grain 2, **b** von-Mises stress response on different grains, and deformation activities is shown for **c** twin, **d** basal, **e** prismatic and **f** pyramidal slip systems

result of twinning in grain 1 and grain 2. The stress relaxation due to twin formation in grain 1 and grain 2 is responsible for the stress drop that results in plateau region in stress–strain curve. Figure 2c shows the effects of accumulated shear in grain 3 due to twinning in grain 1 and grain 2. Likewise, the plastic strain carried by twin tip in the grain boundary of grain 3 is accommodated by basal, prismatic, and pyramidal $\langle c+a \rangle$ slip systems as seen in Fig. 2d, e, and f respectively.

The twin variant in grain 2 is different from the twin variant nucleated in grain 1. The stress carried by twin in grain 1 resolved to both (0 $\bar{1}$ 1 2) [0 1 $\bar{1}$ 1] and (1 $\bar{1}$ 0 2) [$\bar{1}$ 1 0 1] twin systems show that resolved shear stress for (1 $\bar{1}$ 0 2)[$\bar{1}$ 1 0 1] twin variant is significantly higher than other twin variants including (0 $\bar{1}$ 1 2)[0 1 $\bar{1}$ 1] that twinned in grain 1. The nucleation of different twin variant as a result of twin accommodation at grain twin boundary has been previously observed in experiments [44].

With the implementation of characteristic twin spacing and site-specific twin nucleation criterion using hydrostatic pressure, we are able to reproduce the twin-lamellae induced microstructure that is observed in real experiments. Although the current model is not complete and has many limitations, this path for twinning criterion with multiple twins in crystal plasticity models is groundbreaking and should be evolved.

Conclusions

This work incorporates the characteristic twin spacing mechanisms observed in twinning-induced microstructure with site-specific twin nucleation criterion based on hydrostatic stress. Twinning process is a combination of twinning shear glide and shuffle mechanisms. This work makes an effort to include shuffle mechanism, which is a diffusion process that depends on hydrostatic stress, in a crystal plasticity framework to accurately incorporate the role of twinning in microstructure evolution, hardening, and damage initiation. The model can reproduce the multiple twins' nucleations with characteristic twin spacing, and butterfly-like twin structure at the grain boundary as a result of different twin variants nucleating on opposite sides of the grain boundary.

Acknowledgements Research was sponsored by the Army Research Laboratory and was accomplished under Cooperative Agreement Number W911NF-15-2-0025. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the Army Research Laboratory or the US Government. The US Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright notation herein.

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