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Numerical study of the stress state of a deformation twin in magnesium

M. Arul Kumar,[a,*] A.K. Kanjarla,[b] S.R. Niezgoda,[c] R.A. Lebensohn[a] and C.N. Tomé[a]

[a] *Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[b] *Department of Metallurgical and Materials Engineering, Indian Institute of Technology (IIT) Madras, Chennai 600036, India*
[c] *Department of Materials Science and Engineering, The Ohio State University, Columbus, OH 43210, USA*

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Abstract—We present here a numerical study of the distribution of the local stress state associated with deformation twinning in Mg, both inside the twinned domain and in its immediate neighborhood, due to the accommodation of the twinning transformation shear. A full-field elastoviscoplastic formulation based on fast Fourier transformation is modified to include the shear transformation strain associated with deformation twinning. We have performed two types of twinning transformation simulations with: (i) the twin completely embedded inside a single crystal and (ii) the twin front terminating at a grain boundary. We show that: (a) the resulting stress distribution is more strongly determined by the shear transformation than by the intragranular character of the twin or the orientation of the neighboring grain; (b) the resolved shear stress on the twin plane along the twin direction is inhomogeneous along the twin–parent interface; and (c) there are substantial differences in the average values of the shear stress in the twin and in the parent grain that contains the twin. We discuss the effect of these local stresses on twin propagation and growth, and the implications of our findings for the modeling of deformation twinning.
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Keywords: Deformation twinning; Hcp materials; Twinning shear transformation; Crystal plasticity; Local stress distribution

1. Introduction

Plastic deformation in materials with hexagonal closed-packed (hcp) crystal symmetry is usually achieved by a combination of dislocation glide and deformation twinning. Unlike dislocation glide, which reorients the lattice gradually, {10–12} tensile twinning in Mg is characterized by a localized shear transformation and a nearly 90° reorientation of the *c*-axis in a small domain of the crystal. As a consequence of this transformation there is an important stress re-accommodation in the vicinity of the twin, which affects further twin propagation.

Deformation twinning in hcp materials can be rationalized as a three-step sequence: nucleation, propagation and growth (see Fig. 1), and the mechanisms controlling each of these steps are different. Nucleation refers to the process of formation of twin nuclei, and recent molecular dynamics studies suggest that this is a very local phenomenon involving reactions between grain boundary dislocations and stress-driven slip dislocations, combined with atomic shuffling [1–4]. Molecular dynamics results concerning grain boundary nucleation processes were introduced in statistical models, which also include stress fluctuations for deciding which, if any, twin variant is activated in a given grain [5–7].

Propagation refers to the process of the twin front moving into the bulk of the grain and eventually encountering a grain boundary, or an obstacle inside the parent crystal, such as another twin. This paper is focused on elucidating the stress field that develops at the end of the propagation phase when: (i) the twin is completely embedded in its parent grain or (ii) the twin front is arrested at a grain boundary. In the first case, we study the local stress distribution without any misorientation ahead of the twin front, while in the latter case a significant misorientation may be present in the vicinity of the twin front. In this way, we get insight into how the stress field depends on the misorientation across the grain boundary at which the twin was arrested.

Growth is the process through which the twin interface advances inside the grain and provides significant plastic shear. While growth is driven by the resolved shear stress at the twin–parent interface, such a local state is not available when using effective medium homogenization models based on the inclusion formalism. As a consequence, different assumptions are made regarding the stress state that induces twin growth in such homogenization models [8,9]. The present study sheds light on this important aspect of twinning modeling.

Recent statistical electron backscatter diffraction (EBSD) and modeling studies of deformed Mg and Zr [6,10–12] attribute the frequently reported presence of twin

* Corresponding author; e-mail addresses: marulkr@lanl.gov; marulkr@gmail.com

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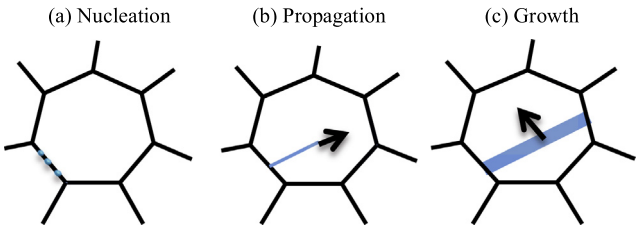

Fig. 1. Schematic of the three steps involved in the deformation twinning process. (a) Nucleation: formation of twin nuclei at the grain boundaries. (b) Propagation: transformation of a stable twin nucleus into a lenticular twin propagating towards the other side of the grain. (c) Growth: increase of twin thickness upon further strain.

variants with low Schmid factor to a local-stress-controlled nucleation process. In addition, these authors report a correlation between twin thickness and high Schmid factor that they attribute to the fact that better oriented twins can more easily overcome the back-stresses that we explore in this paper. Moreover, small-strain cyclic experiments performed on Mg alloys by Lou et al. [13] and Wu et al. [14] highlight the role played by de-twinning in accommodating reverse deformation, and suggest that de-twinning is strongly dependent on the local stress states previously induced by twinning.

Experimental measurement of local stress states in polycrystalline materials, which would provide ultimate validation to the simulations reported here, is not a trivial task. Surface-based techniques such as digital image correlations (DICs) measure some components of the local plastic strain tensor on the surface of deforming materials, but they do not provide measurements of the elastic strain components needed for calculating the stress tensor [15]. Attempts at using the cross-correlation EBSD technique to measure the elastic strain tensor on the surface of the deformed polycrystalline material proved futile due to the extremely high sensitivity of strain error of the technique to the local spin tensor and diffraction geometry, leading to unrealistic values of elastic strains [16–19]. Recent advances in cross-correlation show progress in this area and such measurements may be possible in the future [20].

Also relevant to the present study are recent advances in high-energy X-ray synchrotron experiments, particularly the far-field three-dimensional X-ray diffraction (3-D XRD) techniques that allow one to measure in situ the average elastic strain in a bulk grain. Aydiner et al. [21] employed this technique to monitor the average stress state of a bulk grain and a newly formed deformation twin inside it in AZ31 alloy. Their experiment provides insights into the physics of deformation twinning: upon nucleation, the average value of the resolved shear stress on the twin plane along the twin direction was not only different but of opposite sign in parent and twin. This stress reversal was interpreted to be a consequence of the back-stress induced by internal constraints imposed by the neighboring grains in response to the localized shear associated with the newly formed twin. More recently, Bieler et al. [22] reported similar results for twins in Ti.

In what concerns the incorporation of twinning into crystal plasticity models, it is clear that there is a need for knowing the stress at the twin–parent interface, since this stress is the one that drives the twinning dislocations and so twin growth. Macro-scale level viscoplastic and elastoplastic effective medium models such as the ones used for Mg by Proust et al. [23] and Clausen et al. [8], respectively, rely on the average stress in the parent for activating the twin. The implicit assumption in such a procedure is the continuity of the shear stress components parallel to the twin–parent interfaces. While such continuity is physically required at the microscale, it does not imply that those particular stress components are constant across the whole grain. As a matter of fact, recent measurements of local elastic strain across parent and twins confirm that elastic strain gradients are present in the vicinity of the twin interface [24]. Moreover, simulations performed by Proust et al. [25] allowed these authors to conclude that predictions of mechanical response upon reload in Mg were more in line with experiments if the condition of average continuity was relaxed. More recently, Wang et al. [9] found that using the average stress associated with the inclusion that represents the twin to calculate the resolved shear on the twin interface leads to results in better agreement with Mg alloys experiments, than when the average stress associated with the parent grain is used.

Crystal plasticity based full field finite element models are capable of predicting the local stress state at the twin–parent interface and that can be used for the twin growth simulation [26,27]. But these models are solved under the framework of continuum mechanics at the macroscale level to capture the stress–strain response, texture and twin distribution. On the other hand, nanoscale level atomistic simulations study the twinning process from the perspective of dislocations interaction with twin–parent or grain boundary interface [1–4]. Both macro scale level homogenization models [8,9,23,25] and full field models [26,27], and nanoscale level atomistic simulations [1–4] fail to capture the local stress state associated with the twinning process at the microscale level, which is experimentally observed by Aydiner et al. [21].

In this paper, we perform local stress calculations at the microscale level in hcp grains using an elastoviscoplastic formulation based on fast Fourier transformation (FFT) [28]. We modify the formulation to simulate the transformation strain associated with deformation twinning. We use a continuum approach to solve the equilibrium equation, and no attempt is made here to introduce dislocation theory at the twin–matrix interface [29]. We study the effect of twinning transformation and neighboring grain crystal orientation on local stress distribution. From this study we conclude that the twinning transformation plays a more important role on the local stress distribution than the neighboring grain orientation. We also study the back-stress induced in the twin and in the parent grain by the reaction of the medium to the twinning shear transformation. We believe that this back-stress should play a relevant role in controlling twinning/de-twinning during cyclic deformation of hcp materials.

2. Numerical method

The FFT-based formulation used here was originally developed by Moulinec and Suquet [30] as a fast algorithm to compute the local and effective mechanical response of composite materials, in which the source of heterogeneity is related to the spatial distribution of phases with different mechanical properties. The FFT formulation was later

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