A Multi-scale Statistical Study of Twinning in Magnesium

C.N. Tomé, I.J. Beyerlein, J. Wang, and R.J. McCabe

Hexagonal close packed (HCP) materials such as Mg, Zr, Ti, and Be are used in automotive, nuclear, aeronautic, and defense technologies. Understanding and controlling the formability of these materials is extremely relevant for these technologies. Such understanding requires an understanding of deformation twinning, an important deformation mechanism in HCP. Here we present a multi-scale modeling paradigm that passes information from the atomistic scale to the mesoscale represented by an individual grain in a polycrystalline metal. The single crystal model is, in turn, integrated into an Effective Medium model, which relates the behavior of all grains in the aggregate to the bulk response, such as stress-strain and texture evolution. This article focuses on application of the multi-scale model to HCP polycrystalline magnesium.

INTRODUCTION

In hexagonal close packed (HCP) materials such as Mg, Zr, Ti, Be, and their alloys, dislocation slip is easiest along the basal compact direction $<11\bar{2}0>$, either on the (0001) basal plane or the $\{10\bar{1}0\}$ prismatic planes. These dislocations, however, cannot accommodate deformation along the c-axis. The alternative shear mechanisms available for doing so are either <c+a> slip on the $\{10\bar{1}1\}$ planes, $\{10\bar{1}2\}$ tensile twinning, or $\{10\bar{1}1\}$ compressive twinning. There are other slip and twinning modes, but the ones mentioned above are the ones most frequently observed. The problem with <c+a> slip is that these dislocations have a large Burgers vector and a non-planar core, which makes their activation energetically unfavorable. Twinning dislocations, on the other hand, have smaller Burgers vectors and propagate more easily. The drawback with twinning is that it is directional (unique sense of shear) and that twin nucleation needs to be activated before any propagation and growth of twins can take place. Nucleation and propagation are two different mechanisms: while twin propagation is driven by long range stress states across grains, twin nucleation is driven by local stress states and local atomistic configurations at grain boundaries. Twinning competes favorably with <c+a> slip when high internal stresses are likely, as in low temperature or high rate deformation. In addition, twinning differs from slip in that twinned domains represent regions of shear localization. As a consequence, in addition to their role as 'shear-accommodators', twins can also act as 'crack initiators' at twin-termination interfaces not capable of transmitting the localized shear (i.e., by emitting dislocations or twins across grain boundaries into neighboring grains).

Clearly, twinning plays an important role in the ductility of hexagonal materials. This paper explains how to account for the fundamental mechanisms of slip and twinning and how to integrate them into a multi-scale approach for predicting the macroscopic response of HCP aggregates. Because twin propagation is responsible for the characteristic hardening and texture evolution in HCP metals subjected to plastic deformation, most twin analyses ignore the preliminary nucleation stage and concentrate only on the twin propagation (thickening) stage. Here a statistical experimental characterization and modeling approach is presented to describe twin nucleation and propagation in HCP materials and apply it to high-purity magnesium. This research highlights the role that micro-scale twin nucleation and local stress states play in determining macro-scale polycrystal response.

How would you…

…describe the overall significance of this paper?

This paper shows, for the case of twinning, how one can link length scales by identifying what is relevant at each scale and by developing strategies for incorporating such information into the next scale. In addition, local variability and heterogeneity inside materials is tackled here using a statistical treatment.

…describe this work to a materials science and engineering professional with no experience in your technical specialty?

Hexagonal materials such as magnesium deform by slip and twinning. Understanding the role played by twinning during plastic deformation is essential if one is to develop reliable forming processes for these materials.

…describe this work to a layperson?

Quantitative predictive models of the plastic response of metallic aggregates represent invaluable tools for the design of parts and for simulating and improving the forming processes.

THE ATOMIC SCALE

Twin nucleation begins at the atomic scale. Using a topological analysis, molecular static/dynamics (MS/MD), and density functional theory (DFT), we studied twin nucleation in HCP Mg, Zr, and Zn.[1–3] The results show that a twin nucleus must consist of at least 6 atomic layers for it to be stable and that a single twinning dislocation cannot glide alone in a perfect HCP crystal, but only on a pre-existing twin boundary plane. The important conclusions from these studies are: the traditional pole mecha-

nism for twin nucleation proposed by Thompson and Millard[4] is not feasible for HCP metals; and twin nucleation is energetically unlikely to occur inside the grain because it involves a zonal dislocation with multiple atomic layers. Experimental electron backscattering diffraction (EBSD) supports the notion that twins always start at grain boundaries.[5–8]

This result led us to examine the atomic structure of symmetrical tilt grain boundaries (STGBs) using MS, and study dislocation-GB interactions using MD.[3] For this we used a reliable interatomic potential for magnesium.[9] The important finding from the MS simulation is that for tilt angles, θ, greater than 28º, STGBs of magnesium can be characterized as an array of low energy coherent boundaries plus grain boundary dislocations (GBDs) (see Figure 1). The Burgers vectors of the GBDs within STGBs are large in comparison to the zonal twinning dislocation, and can potentially react with incoming lattice dislocations or dissociate into partials to produce the defects needed for a stable twin nucleus formation. For a 17º STGB, MD simulations show that the leading dislocation in a pile up reacts with the GB and nucleates a few small $(\bar{1}012)$ twin embryos, which coalesce with time to form a sizable and stable twin nucleus (Figure 1b). For a 68º STGB, we observe migration of the boundary away from the initial position due to the glide of twinning dislocation dissociated from the incoming lattice dislocation (Figure 1c). These results demonstrate that: twins can nucleate from grain boundaries; the grain boundary misorientation, by way of its atomic structure, has a significant influence on the mechanism for twin nucleation; and pile ups constitute a plausible nucleation-triggering mechanism.

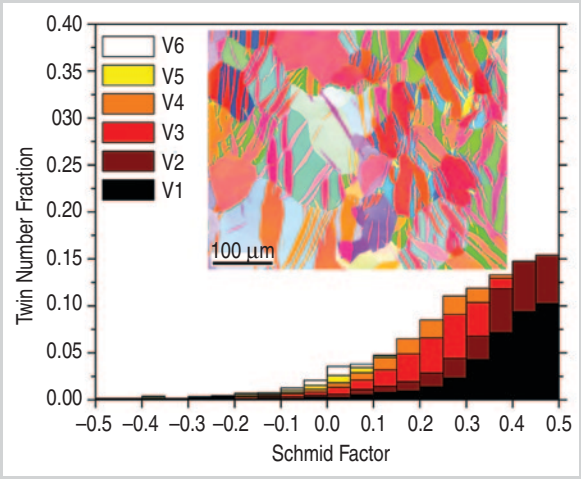
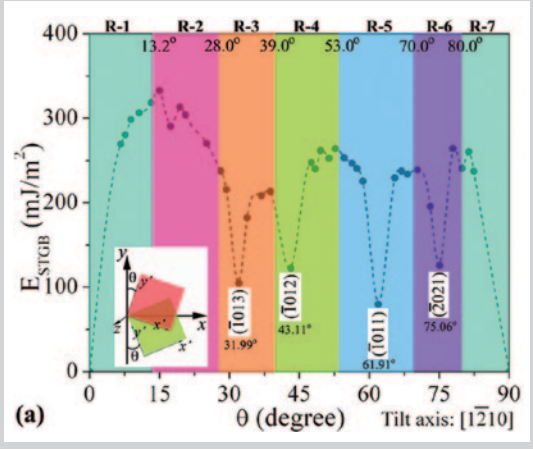


Figure 2. Twin statistics based on EBSD data of rolled magnesium compressed 3% along the in-plane direction. Frequency of twin variants as a function of their Schmid Factor. V1 is the variant with the highest SF in a grain, and V6 the one with the lowest SF.



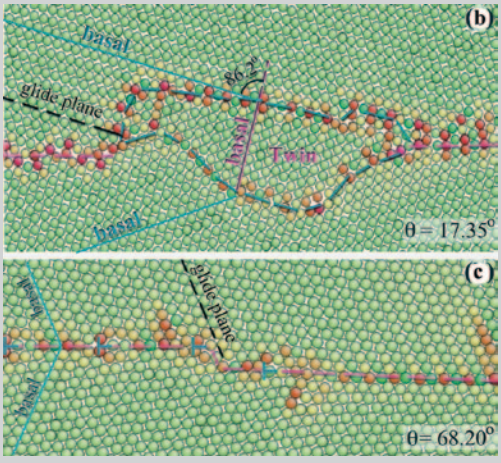


Figure 1. (a) Excess potential energies of grain boundaries as a function of tilt angle θ. The seven regions R-1 to R-7 mark ranges of θ in which STGBs can be viewed as having similar atomic structure. R-1 and R-7: arrays of GBDs; R-2: random configuration STGBs; R-3 to R-5: twin boundaries plus GBDs; R-6: {$\bar{2}$021} STGB plus GBDs. Interaction between STGBs and a four-dislocation pileup: (b) twin nucleation at a 17.35º STGB; (c) migration of a 68.20º STGB twin boundary. Dashed lines in (b) and (c) outline the boundaries.

MESOSCALE STATISTICAL ANALYSIS

The atomistic simulations of tilt boundaries described above suggest a possible twin nucleation mechanism, but refer to very specific tilt configurations. In parallel, we carried out an experimental statistical analysis of grain boundaries and twins. A computer code was developed[10] to derive a suite of twin statistics based on raw EBSD data. The statistics produce correlations between twinning characteristics (such as the presence of twins, number of twins, twin thickness, twin type, twin variant) and grain characteristics (such as orientation, size, and neighbor grain parameters). Using this code we analyzed EBSD scans comprising thousands of grains and {10$\bar{1}$2} tensile twins in magnesium (see Table I). In what follows we discuss twinning statistics for magnesium deformed 3% at 300K.[6]

The Schmid factor (SF), defined as the ratio between the resolved shear

Table I. Number of Features Sampled in EBSD Micrograph of Magnesium Deformed 3% In-plane Compression

Feature	Mg 3%
Number of Grains	2,340
Number of Twins	8,550
Number of Twinned Grains	1,534
Number of Grain Boundaries	11,698

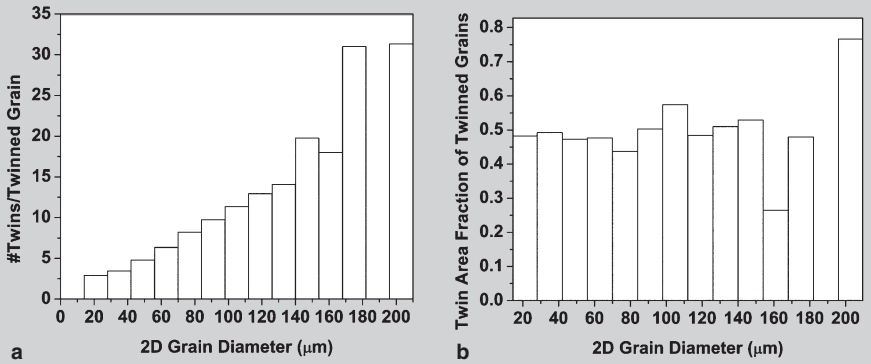


Figure 3. Magnesium deformed 3% IPC. (a) Number of twins per grain and (b) twinned volume fraction per grain, plotted versus grain diameter.

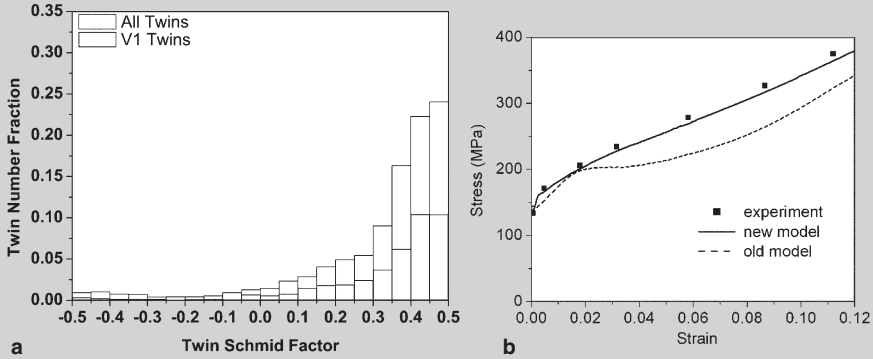


Figure 4. Simulated in-plane compression of magnesium at 300K. (a) Frequency of twin variants (Variant 1 against the rest) as a function of the twin Schmid factor. (b) Measured (symbols) and predicted (lines) stress-strain response. The solid line is obtained when twin propagation is subordinated to previous nucleation driven by stress fluctuations. The dashed line corresponds to considering only twin propagation in the simulation.

stress on the twin plane and the value of the macroscopic compressive stress, provides a geometric measure of how well a twin system is oriented with respect to an external axial stress. The SF of observable twins is the most usual parameter quoted in association with twinning, especially when discussing whether twin activation obeys a "Schmid criterion." In our analysis, the tensile twins observed in any given grain in the EBSD were classified as variant 1 to 6, in decreasing order of their SF. If twins obeyed a Schmid criterion, the twins observed would mostly be those corresponding to variant 1. This is not always the case, however. Figure 2 shows the measured fraction of twins of each variant, as a function of the SF of the variant: only about 40% of them correspond to variant 1, and some of the observed twins have very low SF. The reason is that while the classification by variants is based on the macroscopically applied stress, twin nucleation is controlled by local stresses, which may be different.

Another frequently discussed characteristic of twinning is whether a Hall–Petch effect applies to it, that is, if twinning is easier to activate in larger size grains. Our analysis of magnesium and zirconium indicates that, at least in aggregates with a grain size distribution covering two orders of magnitude, a Hall–Petch effect is not observed. Figure 3 supports this assertion: while larger grains contain more twins (Figure 3a), the volume fraction of twins is insensitive to the grain size (Figure 3b).

Many conclusions follow from the EBSD statistical correlation analysis of twins in magnesium and zirconium.[5,6] Among the most important are: the twin variant with the highest Schmid factor is not always the one that nucleates; twin thickness and twin fraction are independent of grain size, which negates the frequently postulated Hall–Petch effect for twinning; low angle grain boundaries exhibit a higher probability of twin nucleation; and twin nucleation is driven by local (micro) stresses, but twin propagation is driven by the resolved shear stress associated with longer range inter-granular stresses.

MESOSCALE STATISTICAL MODELING

To date, the constitutive laws used for describing twinning do not account for its statistical nature. The onset of twinning has been most often modeled by a deterministic strain or stress-based criterion that tends to favor the variant 1 twins, and commonly used criteria result in twinning in all grains of the same orientation at nearly the same strain. Consequently, under conditions that favor profuse twinning (e.g., low temperature, high strain rates, certain crystal orientations), the constitutive model overestimates the evolution rate of twin volume fraction and texture, and inaccurately simulates the flow stress and hardening rate in the stress-strain response (see lower dashed line in Figure 4b). In addition, models do not introduce a correlation between the number of twins and the grain size, although observations show evidence of such correlation. To improve predictive capability, a probability model for twin nucleation was recently developed[11] which accounts for many of the statistical features characterized by EBSD. The nucleation model

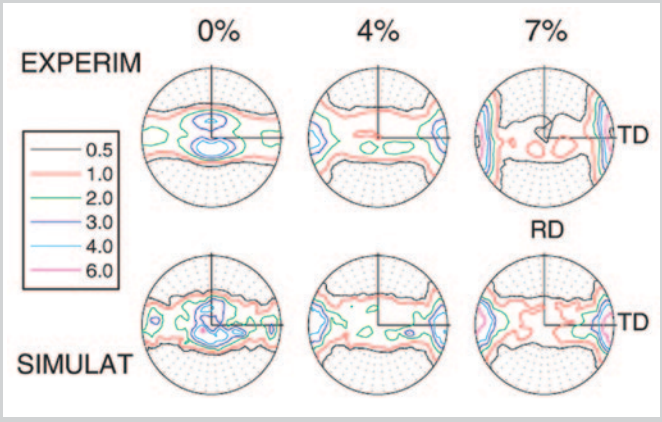


Figure 5. Basal poles (0001). Comparison of experimental and predicted textures in magnesium deformed to 3% and 7% by in-plane compression at 300K. Observe the rapid reorientation of the c-axis along the compression axis (horizontal TD). Notice the good qualitative agreement in the intensity evolution.

is based on the idea that twins originate from statistical distributions of GBDs in the grain boundaries, which may vary in spacing, Burgers vector, and line direction. In this model, the number of GBDs that are transformed under stress into twin nuclei is described by a stochastic Poisson process and the rate of this process increases with both local stress and grain boundary surface area. As either factor increases, the rate of nucleation increases. Based on this discrete description, the formulation develops a continuous distribution of threshold stresses for nucleation as a function of grain boundary size and misorientation angle. A separate numerical algorithm can then sample nucleation stresses from this distribution (using a random number generator) and assign them to material 'elements' (e.g., model grains or grain boundaries). Nucleation occurs when the local stress state, the sum of the applied and internal stress states, resolved on a given twin variant first exceeds the statistically assigned nucleation threshold stress. In this way, for a bulk polycrystal under a prescribed loading condition, the nucleation model dictates when nucleation occurs, in which grains, with which variant, and the number of twins. Subsequent growth of the twin variants nucleated is treated by a separate model, which is controlled by a Schmid criterion and unlike nucleation, is assumed deterministic. Another important difference is that the stress state that drives growth is considered to be the long-range stress state prevailing over the grain interior. Because nucleation is governed by short-range stress states at the grain boundaries and growth by long-range stresses in the grain, grain orientation affects twin growth more strongly than twin nucleation. When implemented into an Effective Medium model the nucleation model predicts variability in the selection of twin variants and broadens the interval of macroscopic strain over which twins nucleate and propagate, yielding stress-strain curves, twinning statistics, and texture, in agreement with experimental measurement.

MESOSCALE CONSTITUTIVE RESPONSE OF THE GRAINS

The twin nucleation model predicts which twin variant will nucleate, if any at all, in a given grain. The nucleation criterion is based, among other things, on fluctuations in the average stress state in the grain. Grain scale models are needed to evaluate such stress. We use a composite grain (CG) model to represent the barriers that twins present to the propagation of dislocations,[12–14] and we use a dislocation-density (DD) hardening law to relate the critical stress to activate slip dislocations with the evolution of dislocation densities of different slip modes.[15] In the CG model each grain is treated as a layered structure of twin-matrix domains (as in EBSD inset in Figure 2). The CG model follows the evolution of twin fraction in each individual grain, captures the directionality of the barriers that twins present to dislocation propagation, and the evolving morphology of twins from thin to thick lamellae. The DD hardening law uses dislocation densities for each deformation mode as a state variable. The activation of the different slip modes is a function of temperature and strain rate. The resistance to slip is the result of the storage of forest and substructure dislocations, and their interaction with twins. The capability of the model to predict hardening and texture evolution in Zr, Mg, U, and Be, under temperature and strain path changes has been reported in References 15–19.

MACROSCALE CONSTITUTIVE RESPONSE OF THE AGGREGATE

The three mesoscale models—statistical twin nucleation, composite grain, and dislocation density evolution—were integrated to provide a constitutive model for an HCP grain that may deform by slip and twinning. This integrated model for the individual grain was, in turn, implemented into a macroscopic Visco-Plastic Self-Consistent (VPSC) polycrystal plasticity code,[20] which simulates the hardening and texture evolution of aggregates during plastic deformation. VPSC represents the aggregate as a collection of grains (crystal orientations) with volume fractions that are consistent with the initial texture of the material to be simulated. Deformation is accommodated by crystallographic slip and twin shears, $\dot{\gamma}^s$, inside the grains. The strain rate of the grain is given by a visco-plastic law, representing the sum of shears in all active slip and twinning systems

$$\dot{\varepsilon}_{ij} = \sum_s m^s_{ij}\dot{\gamma}^s = \dot{\gamma}_0 \sum_s m^s_{ij}\left(\frac{m^s_{kl}\sigma_{kl}}{\tau^s}\right)^n \quad (1)$$

Here m^s_{ij} is the geometric Schmid tensor for system s, σ_{kl} is the stress tensor inside the grain, and τ^s is the threshold stress for activating the system. The variation of τ^s with strain determines the macroscopic hardening, and the distribution of $\dot{\gamma}^s$ determines the texture evolution of the aggregate. Within VPSC each grain is treated as an ellipsoidal visco-plastic inclusion embedded in and interacting with a visco-plastic effective medium that represents the polycrystal. The response of the polycrystal is given by the average response of the grains. For each strain increment in a given strain path, VPSC calculates a homogeneous grain stress for every grain in the aggregate that in general deviates from the macroscopic applied stress state. This grain stress adequately represents the stress states that would drive twin growth but not twin nucleation. It does not account for the spatially varying stress states near the grain boundaries where twins originate. The latter would lead to a local resolved shear stress on each twin variant, which for the calculations below is modeled by a uniform random distribution.

COMPARISON WITH EXPERIMENT

The multi-scale approach described above was applied to high-purity zirconium and magnesium, the two HCP materials that were statistically characterized using EBSD.[11,21] Here, we only report some of the simulation results for magnesium, where we made available $(0001)<11\bar{2}0>$ basal slip, $\{10\bar{1}1\}<\bar{2}113>$ pyramidal slip, and $\{10\bar{1}2\}<\bar{1}011>$ tensile twinning.

In Figure 4a we report the predicted distribution of twin variants after 3% deformation. Observe that only about 40% of the twins are of variant 1, and that twins with very low Schmid factors are predicted to be active. Both features are quantitatively consistent with EBSD measurements. In this case limits of the uniform distribution from which stress fluctuations are sampled were set to ±9 MPa. As a result, stress concentrations at the time of nucleation varied widely

from 1.0 to 4.0. If the fluctuations were not considered, then over 95% of the twins nucleated would be variant 1. Therefore, the predictions suggest that stress fluctuations generated at grain boundaries are responsible for observed dispersions in twin variant selection.

Also in Figure 4 we compare the current model predictions (solid lines) with the measurement (symbols) and with a version of the model that employs a deterministic twin nucleation criterion where fluctuations are not allowed. In the latter, twinning occurs simultaneously at the onset of deformation in several grains, which induces a horizontal plateau (zero hardening rate) within the initial 4% strain (dashed line in Figure 4b). In contrast, in the probability-based model, twinning occurs statistically throughout the polycrystal over a wider strain interval. As a result, there is a spread in nucleation events along the strain path, a spread in the variant selection as a function of grain orientation, and a dispersion in the number of twins per grain. The consequences are that the hardening increases monotonically (Figure 4b) and texture evolution takes place in a more gradual and diffuse manner (Figure 5). Both results are in agreement with measurements. The statistical details of twinning at the microscale have measurable effects on the deformation behavior of the material at the macroscale.

Recall that the nucleation model dictates the twin variant nucleated and the growth model determines which twin nuclei expand to a visible size. As a result, lower rank twin variants that happen to nucleate because of a high stress fluctuation are not likely to grow as thick as the higher rank variants. Significantly, this distinction leads to texture predictions in agreement with bulk neutron diffraction measurements (Figure 5), and twin thicknesses and total twin volume fractions in agreement with EBSD. Although not shown here, the model also captures well the strong grain size effect in the number of twins formed per grain observed in EBSD (Figure 3b). Overall we conclude that modeling the variability associated with the stochastic twinning process is critical for correctly predicting the evolution of the flow stress, hardening rate, texture, and twin volume fraction with strain.

CONCLUSIONS

Twinning plays as important a role as slip in determining the plastic properties and plastic response of HCP aggregates. While twin propagation is responsible for accommodating shear and for rapid hardening and texture evolution, the frequently ignored process of twin nucleation must obviously occur first. In addition, because twin nucleation is controlled by local atomistic configurations and stress concentrations at grain boundaries, the modeling of HCP plastic forming requires a multi-scale approach to capture the plastic response. Here we describe such an approach that includes a sophisticated stochastic model for twin nucleation, the effect of twin barriers upon dislocation propagation, the evolution of dislocation densities in basal and pyramidal systems, and an Effective Medium approach for describing grain interactions and average aggregate response. The use of atomistic modeling and statistical characterization of twinning by EBSD provides correlations between twins and grain features, which are required for supporting and guiding any modeling development effort. An important statistical distribution conditioning nucleation, which presently we treat in ad-hoc manner, is the one of local stresses associated with grain boundaries. We envisage to use, in the future, high resolution EBSD[22] and local field simulations[23] in the vicinity of grain boundaries, to derive experimental and numerical characterizations of such stresses.

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