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Viewpoint article

Modeling discrete twin lamellae in a microstructural framework

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ABSTRACT

The impact of deformation twins on the mechanical response of metals derives from the fact that they are microstructural inhomogeneities that create lattice reorientation and introduce local stress fields. Efforts have begun towards microstructural modeling of discrete twin domains within individual grains and the stress and strain fields that result from them. The aim of this viewpoint article is to review these endeavors, highlighting the insights gained by these studies, the advantages and disadvantages of the seemingly diverse approaches taken to date, and on this basis, offer our perspective on promising future steps.

Twinning is one of the basic deformation mechanisms by which individual crystals accommodate mechanical strain [1,2]. Deformation twins are discrete domains that are believed to begin as atomic scale embryos that grow with applied strain to become grain-scale lamellae. Twin domains are crystallographically reoriented with respect to the parent grain, which introduces a boundary between parent and twin domain a 'twin boundary'. Formation of a twin shears the material by a characteristic amount, the twin shear, on the twin plane and in the twinning direction [1,3,4].

Plastic deformation in polycrystalline metals is most often accommodated by plastic slip, but under certain circumstances can be carried by both twinning and slip. These conditions are specific to the material and twin mode, but generally twinning is reported to occur easily at high loading rates, low temperatures, and under particular states of strain [1,5,6].

The macroscopically observed stress-strain response is radically different when twinning and slip together accommodate plastic deformation than when plastic slip acts alone. Fig. 1 shows examples of the tension-compression asymmetry that can arise in materials that twin readily under ambient pressures and quasi-static rates. These metals possess a low symmetry crystal structure and are α-titanium (α-Ti) [7], α-zirconium (α-Zr) [8], a magnesium alloy (AZ31) [9], and α-uranium (α-U) [10]; all results are obtained from sheet material with a strong texture. Due to the choice of applied load direction relative to the sheet texture and allowed deformation modes, in each of the tension cases, deformation was accommodated by slip, whereas in compression it was accommodated by slip and twinning. In the predominantly slip (tension) curves, the hardening rate reduces with applied strain, while in the twinning and slip (compression) curves, there are inflection points in the hardening rate, and over some periods the hardening rate increases with applied strain.

Arguably many factors could be responsible for the differences seen in the twinning responses but two are worth highlighting: the preferred slip systems and the morphology of the twin domains. For the three HCP crystal systems shown, in the Mg alloy (AZ31) the easiest slip system is basal slip, whereas in α-Ti and α-Zr it is prismatic slip [2,13–15]. In α-U, which has an orthorhombic crystal structure, the easier slip system is floor slip [16–19]. Twin morphologies can be easily seen in EBSD maps, such as those in Fig. 2, which correspond to the compressed materials in Fig. 1. As shown, the twins manifest as discrete domains within a majority of grains. The crystal lattice within the twin domain has significantly reoriented from that of the parent grain and hence both twin volumes and twin boundaries can be easily exposed. Despite length scale differences relative to parent grain size, some key differences can be observed: in Mg, the twins are few and thick; in Zr and Ti, they are many and thinner compared to Mg; in U, the twins are numerous and very thin.

Such morphological details of the twin can locally affect which type of slip is favored and hence influence the macroscopic stress-strain response. The twin introduces a new crystallographic orientation into the grain and within this domain, slip systems can be preferred that are different from those in the parent. The directional boundaries introduced by twins can pose obstacles against slip motion and depending on the relative orientation of the slip mode and twin boundary, the barrier

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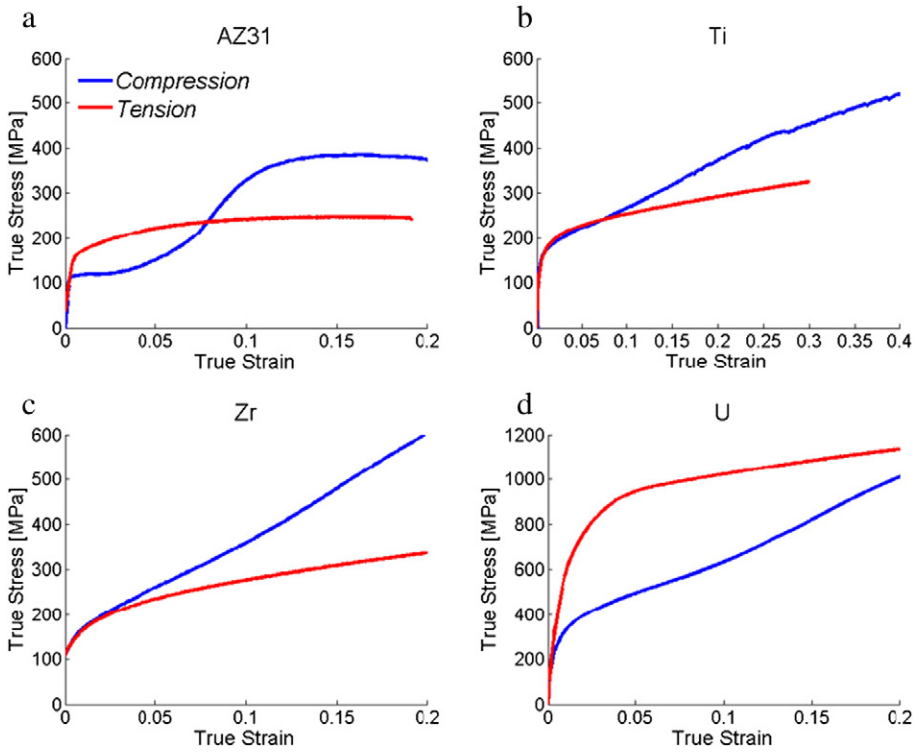

Fig. 1. Effect of deformation twinning on the compressive response of: (a) AZ31 [9], (b) α-Ti [11], (c) α-Zr [12], and (d) α-U [10]. Response in tension for all these metals exhibits characteristics of slip dominated deformation.

can be stronger for one slip system than another. A third way that twin morphology can take affect, which is neglected, is through the local stress states that are generated within the twin and surrounding matrix. The localized stress-strain fields produced by twins, in addition to creating localized hardening, influence local slip activity within the parent grain and twin itself, formation of additional twins, and twin expansion rates [20]. Knowledge of these local stresses and strains could help explain the probability of other twin-related processes, such as twin-twin transmission [21], secondary twinning, and de-twinning [22–24]. Furthermore, through the local stresses that they generate, twins are thought to play a role in recrystallization kinetics [25,26], fatigue, [27], and ductile fracture [28].

To date, we lack a constitutive model that accounts for the changing morphology of the twin, the hardening effect introduced by twin boundaries, and the activation of slip and twinning systems according to the local stresses produced by twins. Most constitutive models for metals that deform by combinations of slip and twinning utilize mean-field polycrystal models, such as Taylor-type [29,30] and self-consistent [31] schemes. In these approaches, the neighborhood is homogenized and hence the grain boundaries and grain neighbors are not explicitly modeled.

Within mean-field codes, four micromechanics approaches currently exist for introducing a reoriented twin phase: (i) predominant twin reorientation (PTR) method [32,33], (ii) volume fraction transfer

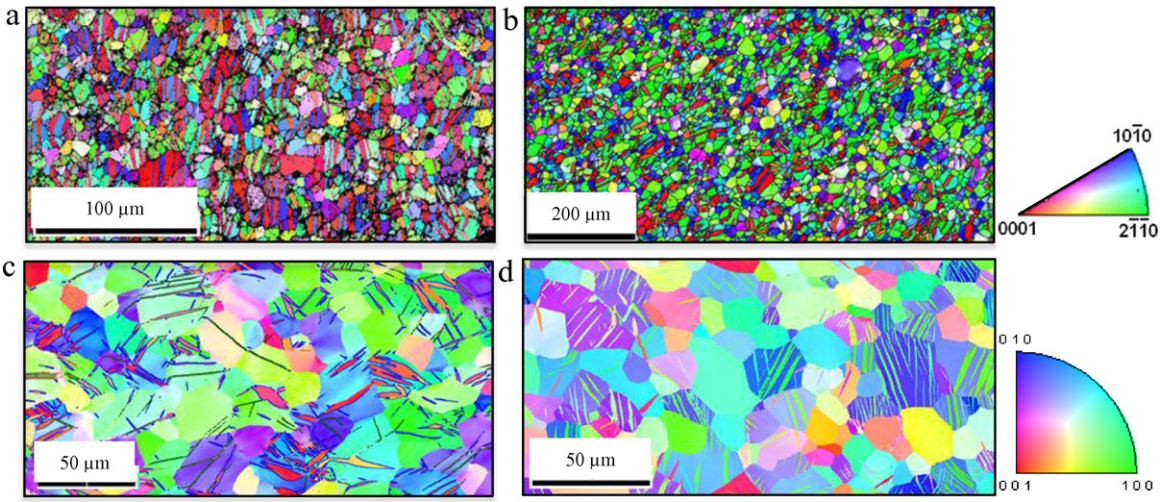

Fig. 2. Inverse pole figure maps showing microstructure evolution in samples compressed along the in-plane rolling direction of sheets of (a) AZ31 to a true strain of 0.04 at 298 K [9], (b) α-Ti to a true strain of 0.1 at 298 K [11], (c) α-Zr to a true strain of 0.08 at 76 K [12], and (d) α-U to a true strain of 0.05 at 298 K [10]. These maps indicate the orientation of the compression axis with respect to the crystal reference frame.