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Direct numerical simulation of deformation twinning in polycrystals

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ABSTRACT

The ability to directly simulate the formation of twin domains in crystalline materials is of interest to the mechanics of materials community. While extensive work has been published on homogenized crystal mechanics treatments of twinning, publications that directly capture twin domain formation are relatively rare. This is due both to the complexities of model development and to the computational costs involved. We present results from simulations of twinning in polycrystals with finite elements that spatially resolve twin formation. Effects of interest include the role of stress concentrations in twin initiation, the interactions among twin systems, and competition between deformation twinning and dislocation glide plasticity. We anticipate that results from models that spatially resolve twin formation will help to inform more homogenized multiscale schemes. We show basic features of the model via numerical simulations on a model polycrystal system in simple shear, and also examine the complete model through large scale simulation of a dynamically compressed polycrystal. Comparisons are made between experimental data from far-field high energy diffraction microscopy (HEDM) and numerical simulations for a magnesium alloy polycrystal in compression. We finish with some final remarks and directions for future work.

1. Introduction and background

Mechanical twinning plays an important role in the plastic deformation of many crystalline materials. Low symmetry crystals in which dislocation mediated slip does not readily accommodate general deformation modes are especially prone to twinning. For example, in hexagonal close-packed (HCP) crystals, slip may be restricted to a relatively small number of basal or prismatic slip systems, and there may not be any readily activated crystallographic slip systems that allow deformation along the c-axis. General loading conditions will therefore tend to produce a combination of deformation by twinning and slip. Additionally, even in high symmetry crystals with ample slip systems such as face centered cubic (FCC) and body centered cubic (BCC) crystals, it is well known that low temperatures and/or high strain rates tends to promote deformation twinning [1,2,3,4]. For example, in BCC tantalum, it is postulated that twinning occurs when the strain rate is sufficiently high that the usual dislocation mechanisms do not provide rapid enough relaxation to prevent the stress from building. There is also experimental evidence to suggest a complex interplay between dislocation density evolution and deformation twinning found in BCC tantalum [4], making tantalum a very interesting material to consider. In what follows, our focus will be concentrated on HCP magnesium alloy AZ31, as well as BCC tantalum.

In modeling the plastic deformation of polycrystalline materials several forms of "crystal plasticity" are in use, such as Visco-Plastic Self Consistent (VPSC), Visco-Plastic Fast Fourier Transform (VPFFT), Elastic-VPSC, Elastic-VPFFT, and full Finite Element (FE) based methods [5,6,7]. There are also numerous partial differential equation solution methods in addition to typical finite element methods, such as the Fast Fourier Transform (FFT) based schemes [8,9], and also a wide literature using phase-field methods [10], although much of the phase-field methods have been for phase transformations [11].

Crystal plasticity based models were initially driven by the

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seminal contributions of Taylor and Schmid [12,13] based on early qualitative observations. Quantitative analysis of slip-based plastic deformation is feasible by a number of constitutive models [14,15]. While slip-dominated crystal plasticity has been widely studied and generally accepted, many questions still exist for twinning. For example, open questions remain regarding twin initiation and the interactions among twins and obstacles. Such obstacles include other twins, grain boundaries, dislocation networks, and so on. Nevertheless, deformation twinning has been incorporated into models that include the combined effects of twinning and slip as inelastic mechanisms (for example [16], and references therein for recent examples). A more complete understanding of such interactions should lead to improved constitutive models and predictive simulation capabilities.

In regard to constitutive modeling of twinning within the crystal plasticity context, one of the earlier contributions was made by van Houtte [17] where it was postulated that twinning could be modeled by reorienting the twinning grain. However, it was shown later that numerous grains are required for such an assumption to obtain reasonable results for a polycrystal calculation [18]. Kalindindi [19] proposed a constitutive model in which twinning was modeled in a manner analogous to slip, and dislocation slip was considered in both the parent and child (twinning-produced) grains. Later Staroselsky and Anand [20] developed a constitutive model for HCP metals based on Van Houtte's criteria for reorientation due to twinning in addition to a modified flow rule to account for grain boundary plasticity accommodation. The model was shown to simulate the average stress-strain response as well as texture in magnesium rods and plates. Typically, these types of modeling efforts do not spatially resolve twin dominions, but rather track a homogenized quantity, such as the twin volume fraction at a material point. Additionally, a few other research groups [21,22,23] have devised and implemented schemes based on evolving an orientation distribution function including the nonlocal contributions from mechanical twinning. However, these types of schemes also do not spatially resolve individual twin domains.

In addition to finite element based approaches to polycrystal plasticity, the self-consistent approach is also prevalent in the literature, and worth mention here. Self-consistent type approaches have also shown great success in describing the deformation of polycrystals when slip is the dominant mechanism of inelasticity and these methods have been extended to include twinning as well [24,25]. The underlying assumption is that each grain may be treated as if it were embedded in a homogeneous effective medium (HEM) which is meant to represent the polycrystal. Then using an Eshelby approach [26] with appropriate analysis the stress-strain response of the grain may be related to the macroscopic response of the HEM. However, means of effectively including the spatially localized nature of twinning in such frameworks is an active area of research [27,28,29,10,30,31], and for that reason we use a finite element based approach in this work.

Multiscale modeling approaches have seen increased popularity and utility in recent years, and we have pursued both concurrent and information-passing types of multiscale models in previous work [32,33,23,34,35,36]. Our multiscale approach in Ref. [36] makes use of an information-passing paradigm: simulation results from lower length-scale calculations are used to define functional forms and parameters at the next larger length-scale. This approach is in contrast with direct (concurrent) multiscale embedding, which is sometimes employed when unit mechanisms are difficult to identify or a stronger coupling between scales is required [32,33,23,34,35]. Much of our previous modeling work assumed dislocation motion as the dominant mechanism for inelasticity with hardening arising from the interactions among dislocations. In this work, we focus attention to direct numerical simulation of twin domains at the crystal level.

Capturing the correct twin domain structure in a model would enable.

- Examining sub-grain level stress heterogeneity and corresponding effects on twinning.
- Capturing autocatalytic effects — twins running into boundaries producing stress concentrations that cause twinning on the other side of the boundary.
- Capturing intra-grain transitions in microstructure due to twinning.
- Informing more homogenized phenomenological crystal models or macroscopic models.
- Creation of a computational capability that allows for model validation by direct comparison with *in situ* grain-resolved X-ray diffraction data that resolves twin domains.
- Examining anisotropic effects in twin formation resulting from changes in deformation mode.

Our objective in this work is to report on our simulations that spatially resolve twin domains and to compare our crystal level simulations with experimental data. Additionally, we discuss how our results could effect higher-scale constitutive theories in a multiscale scheme. Indeed, we anticipate that the incorporation of such crystal level effects into a multiscale strength model will provide additional details to better predict material response in real-world applications.

The remainder of the paper is organized as follows. In Section 2 the basics of the crystal level constitutive model are summarized. In Section 3, using tantalum as an example, we provide an overview of the capabilities of the constitutive model. Specifically Section 3.1 provides model details for tantalum, and Section 3.2, via numerical simulation, shows the basic constitutive model behavior for an idealized tantalum system. That is followed by Section 3.3 where we present a large scale simulation of a tantalum polycrystal. As discussed in Ref. [4], these results for tantalum capture interesting aspects of experimentally observed behavior. A comparison between high energy diffraction microscopy data and simulations for a magnesium alloy is presented in Section 4. And lastly, we finish with some concluding remarks in Section 5.

2. Review of the constitutive model

The model allows for deformation by thermo-elastic lattice distortion, lattice rotation, dislocation based slip, and twinning [37,38,39]. All deformation modes can occur in both the parent and twin domains. In the simulations that follow, BCC tantalum is modeled with twelve $\{1\bar{1}0\}\langle 111\rangle$ slip and twelve $\{211\}\langle\bar{1}11\rangle$ twinning systems.[1] Further, HCP magnesium alloy AZ31 is modeled with three basal $\{0001\}\langle 1120\rangle$, three prismatic $\{1\bar{1}00\}\langle 1120\rangle$, and six pyramidal $\langle c+a\rangle\{11\bar{2}2\}\langle\bar{1}\bar{1}23\rangle$ slip systems, as well as six $\{10\bar{1}2\}\langle\bar{1}011\rangle$ "tensile" twinning systems. More slip systems can be used to model pencil glide type behavior. In most publications related to the modeling framework [37,38,39] the reference rates for the dislocation slip based deformation modes have been fixed. In other crystal level work [40], these rates have been made to depend on the current dislocation density, more like what is done in certain models meant for high rates, for example [41,42,43]. Such considerations can influence slip/

[1] In Section 3.2, we limit the material to a single twin system so that we may more clearly understand the behavior of the constitutive model in a simplified setting.