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Stochastic modeling of twin nucleation in polycrystals: An application in hexagonal close-packed metals

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ABSTRACT

Twinning in hexagonal close-packed (hcp) metals is a multi-scale process that depends on the microstructural and mechanical response details at the polycrystalline aggregate, grain, micro, and atomic scales. Twinning can generally be regarded as a two-step process, a nucleation event followed by propagation and growth. This articles presents a stochastic model for the nucleation of deformation twins in hcp polycrystals. Twin nucleation is modeled through its dependence on lower length scale material details, such as the defect configurations at potential nucleation sites within grain boundaries, and mechanical details such as highly localized stress concentrations at the microscale in a probabilistic manner. These two aspects, the material and mechanical, must align for a successful nucleation event. The nucleation process is cast as a survival model parameterized by the local stress at the grain boundary. The model gives an explicit form for the probability distribution for the critical stress values required for twin nucleation. The model is implemented into a viscoplastic self-consistent (VPSC) crystal plasticity framework in order to test its predictive capability against previously reported statistical characterization in deformed zirconium at multiple temperatures. For implementation in VPSC, the stress concentrations are sampled from a distribution calibrated to full-field crystal plasticity simulations and a three-dimensional model of grain neighbors and distribution of grain boundary areas are implemented.

1. Introduction

1.1. Experimental observations of the statistical nature of twinning

Deformation twinning in hexagonal close-packed (hcp) metals, such as Zr, Mg, Be, Hf, Ti, etc., plays an important role in determining the plastic properties and overall stress/strain response. The growth of twins during deformation is one of the primary mechanisms for accommodating plasticity along the *c*-axis of the individual crystallites and has a dramatic effect on the hardening behavior and texture evolution of the polycrystal as a whole, particularly at room temperature and below. The incorporation of twinning into continuum scale deformation models is difficult in that, from the perspective of the simulation length scale, twinning is a highly variable event. Recent statistical analysis of $\{10\bar{1}2\}$ twinning in hexagonal metals by Capolungo et al. (2009) and Beyerlein et al. (2010) highlight this variability and demonstrate some of the basic features

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which a physics based twinning model must incorporate. These authors found that for Zr, under the same conditions explored in this study, only about 60% of the observed twins were the ones with the highest macroscopic Schmid factor (40% in textured Mg), while the remaining twins were of less favorable variants. Additionally it was observed that, while $\approx 90\%$ of the grains most favorably oriented for twinning contained at least one twin, the remainder did not nucleate. On the other hand, it was also observed that a small, but non-negligible, fraction of grains poorly oriented for twinning (highest Schmid factor in grain $\leqslant 0.2$) did in fact twin. An interesting feature of the quoted statistical analysis is that while the nucleated twin variants deviated from expectation, the subsequent growth of the twins largely followed intuition, in that the twins with higher macroscopic Schmid factors grew to be thicker than twins with lower Schmid factors. This suggests that twin nucleation and the subsequent twin growth are distinct processes that occur at fundamentally different length and time scales.

The nucleation event itself is dependent on the myriad details of the multi-scale material structure (i.e. grain lattice orientation, grain boundary character, defect structures in and near the grain boundary, etc.), as well as the highly local stress state and deformation rate present at the defect structures and internal material interfaces. As a result, the twin density, volume fraction, and morphology can vary widely in grains of the same crystallographic orientation. As such, nucleation is a truly multi-scale event, and from the perspective of the continuum scale, without the benefit of knowledge of the details at the lower length scales, twinning appears to have a large random or stochastic component.

Ongoing research on the possible twin nucleation mechanisms, based on energetic and kinetic considerations, coupled with qualitative or descriptive evidence from optical and electron backscatter diffraction (EBSD) microscopy suggests that twin nucleation occurs at grain boundaries (Beyerlein et al., 2011; Khosravani et al., 2013). Grain boundaries, or other interfaces, are the most likely sources for high densities of partial dislocations, which current nucleation theories require (Wang et al., 2010). Grain boundaries and other defects are the primary locations for stress concentrations in polycrystals, which can supply the energy necessary to overcome activation barriers for nucleation to take place. Additionally, high energy interfaces such as grain boundaries (relative to the bulk crystal lattice) are more likely to be able to accommodate the complex rearrangement necessary to support a stable twin nucleus.

1.2. Challenges in the micromechanical modeling of twin nucleation

The explicit insertion of twin nucleation criteria in polycrystalline mechanical models is problematic in that the actual nucleation event can be considered as a statistically rare microstructure event. In general the term statistically rare microstructure event refers to phenomena where the volume of occurrence is infinitesimal compared to the material volume, or that the probability of observation is virtually zero. The case of a single twin nucleation event in hcp metals can be considered as a statistically rare event in that the nascent twin nucleus forms on a small grain boundary domain which has an area that is vanishing when compared to the entire grain boundary surface in a volume consisting of hundreds or thousands of grains. When considering the very large number of grain boundary segments and strain increments, statistically rare twin nucleation events will still occur thousands of times in the material volume during deformation and, given sufficient time for growth, twinned domains will make up a significant volume fraction of the material.

Crystal plasticity models that incorporate twinning generally do not include a physically based mechanism to account for the observed variability in twin nucleation. As a consequence constitutive models for hcp metals often rely on completely empirical rules to determine when a twin forms, which variant is selected, the number of twins per grain etc. Most models depend on a simple deterministic critical resolved shear stress (CRSS) based law for describing nucleation and subsequent propagation of twins (Salem et al., 2005; Proust et al., 2007; Proust et al., 2009; Abdolvand et al., 2011). The two main problems with CRSS-based approaches are: (1) that the CRSS is typically applied at a length scale (micron to millimeter) several magnitudes larger than the defect scale interactions that trigger twin nucleation and (2) the actual stress to cause twinning is going to be strong function of the myriad details at the atom/defect length scales.

1.3. Objectives of the present work

In this work, we describe an approach to include twin nucleation into constitutive laws for application into crystal plasticity models. This approach is grounded in two underlying assumptions: (1) Twin nucleation, propagation, and growth, are distinct physical processes that are driven by forces acting at different length scales. (2) Twin nucleation is a statistically rare event, which is largely controlled by local atomistic configurations and highly-localized stress concentrations at the grain boundaries. While the model does not explicitly take an atomistic description of the grain boundary into account, the distribution of local structure is implicitly captured in that the critical nucleation strength of a twin is not constant but will adopt a distribution that is an implicit function of the atomistic details of the boundary. The distribution of critical nucleation strengths will be referred to as the material component of twin nucleation and the dependence on local stresses at the grain boundary will be referred to as the mechanical component.To this end we present a stochastic model for twin nucleation, the form of which is largely influenced by the ongoing work in studying grain boundary and interfacial behavior at the atomistic scale. In this model nucleation is not deterministic but instead will occur with a probability that is governed by both material and mechanical factors.